Supplementary Information (SI) for Materials Horizons.
This journal is © The Royal Society of Chemistry 2024

Supporting Information

Reversal Chirality in Solutions and Aggregates of Chiral Tetrachlorinated Diperylene Diimides towards Efficient Circularly Polarized Light Detection

Ke Gao,[#,a] Sang Hyuk Lee,[#,b] Wenkai Zhao,[c] Jaeyong Ahn,[b] Tae Woo Kim,[b] Zhenping Li,[a] Huagui Zhuo,[a] Zhiwei Wang,[a] Xinglong Zheng,[d] Yang Yan,[d] Gang Chang,[e] Wei Ma,[f] Mingming Zhang,[a] Guankui Long,[*,c] Joon Hak Oh,[*,b] and Xiaobo Shang[*,a]

[a]State Key Laboratory for Mechanical Behavior of Materials, Shaanxi International Research Center for Soft Matter, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, P. R. China

[b]School of Chemical and Biological Engineering, Institute of Chemical Processes, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea.

[c]Tianjin Key Lab for Rare Earth Materials and Applications, Smart Sensing Interdisciplinary Science Center, Renewable Energy Conversion and Storage Center (RECAST), School of Materials Science and Engineering, Nankai University, Tianjin 300350, P. R. China

[d]Department of Cardiovascular Surgery, The First Affiliated Hospital of Xi'an Jiaotong University, Xi'an, 710061, P. R. China

[e]Instrumental Analysis Center of Xi'an Jiaotong University, Xi'an, 710049, P. R. China

[f]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049, P. R. China

*Corresponding author. E-mail: xiaoboshang@xjtu.edu.cn (X. Shang); joonhoh@snu.ac.kr (J. H. Oh); longgk09@nankai.edu.cn (G. Long)

[#]Authors Ke Gao and Sang Hyuk Lee contributed equally.

Supplementary Methods

1. Experimental Methods

Synthesis of Chiral Semiconductors and Self-assembly for Nanomaterials: The chiral ((*S*/*R*)-1-cyclohexylethyl) amine were purchased from Tokyo Chemical Industry (TCI). (*S*/*R*/*Rac*)-4Cl-PDI-Cy compounds were prepared according to the literature procedure.[S1] For the synthesis of (*SSSS*)-, (*RRRR*)- and (*Rac*)-4CldiPDI compounds, (*S*/*R*/*Rac*)-4Cl-PDI-Cy (1.34 mmol), CuI (8.03 mmol), L-proline (9.35 mmol), K_2CO_3 (14.72 mmol) in DMSO (25 mL) was heated at 75°C under N_2 for 10 h. The cooled mixture was neutralized with 1M HCl, and extracted with DCM. The organic layers were separated, washed with brine, dried over Na_2SO_4, and purified by column chromatography silica gel, with eluent petroleum ether/DCM = 1:1 to afford (*SSSS*)-, (*RRRR*)- and (*Rac*)-4CldiPDI as black solids. (*RRRR*)- and (*SSSS*)-4CldiPDI NWs were fabricated through bottom-up solution-phase self-assembly. (*SSSS*)- or (*RRRR*)-4CldiPDI (1.0 mg) was dissolved in DCM (2.0 mL) in a 20 mL vial. Then, 2.0 mL of methanol was injected into the solution. After several days, (*RRRR*)- and (*SSSS*)-4CldiPDI NWs were obtained.

Fabrication of Organic Phototransistors (OPTs): Heavily doped silicon wafers (*n*-type, < 0.004 Ω·cm) with thermally grown 300-nm-thick SiO_2 (C_i = 10 nF cm^{-2}) were used as substrates for NWs-OPTs devices. The SiO_2/Si wafers were cleaned with piranha solution for 1 h (a mixture of 70 vol% H_2SO_4 and 30 vol% H_2O_2), followed by UV-ozone treatment. The surface of the wafers was treated with *n*-octadecyltrimethoxysilane (OTS) self-assembled monolayer. OTS solution (3 mM in trichloroethylene) was spin-coated at 1500 rpm for 30 s onto the wafers, and then the samples were kept overnight in a vacuum desiccator with a separate vial containing a few drops of NH_4OH. The wafers were sequentially washed with toluene, acetone and isopropyl alcohol, and dried with nitrogen blowing. The chamber was under high vacuum (< 5.0×10^{-6} torr), and the deposition rate was maintained at 0.2 Å s^{-1}. Gold

source/drain electrodes (40 nm) were thermally evaporated. The source/drain patterns had a channel length (L) of 50 μm and a channel width (W) of 1000 μm (W/L = 20). Fabricated nanomaterials were drop-casted onto OTS-treated SiO_2/Si substrates for NWs-based OPTs. The thin film-based OPTs were fabricated by dissolving (*RRRR*)- and (*SSSS*)-4CldiPDI at a concentration in chloroform (5 mg mL^{-1}) and spin-coating onto a substrate at 2000 rpm. Then the substrates were thermal annealed at 60 °C in a glove box.

Optoelectrical Measurements: The current-voltage characteristics of OFETs were measured inside a vacuum chamber (< 5.0 × 10^{-5} torr), by using a Keithley 4200-SCS semiconductor parametric analyzer. In OPT measurements, monochromatic light was produced using an Oriel Cornerstone 130 1/8m monochromator. CPL illumination was generated through a linear polarizer and a quarter-wave plate (Thorlabs). They were installed between the light source and samples.

Materials Analysis: The ^{1}H NMR and ^{13}C NMR spectra were measured on JNM-ECZ400S (JEOL) 400 MHz or Bruker Avance 600 MHz spectrometer. The absorption spectra were measured using a Cary 5000 UV-vis-NIR spectrophotometer for solution. A Shimadzu UV-vis -NIR scanning spectrophotometer UV-3600 was used to measure absorption spectra for nanomaterials using the diffuse-reflectance method. SEM images were observed using a Hitachi cold SEM microscope. The CD results were obtained using a *J*-815 Spectropolarimeter (JASCO). X-ray diffraction analysis was conducted a Bruker D8 VENTURE PHOTON II MetalJet, in which crystals were frozen in paratone oil inside a cryoloop under a cold stream of N_2. An empirical absorption correction using SADABS was applied for all data. The structures were solved and refined to convergence on F2 for all independent reflections by the full-matrix least squares method using the OLEX2 1.2.

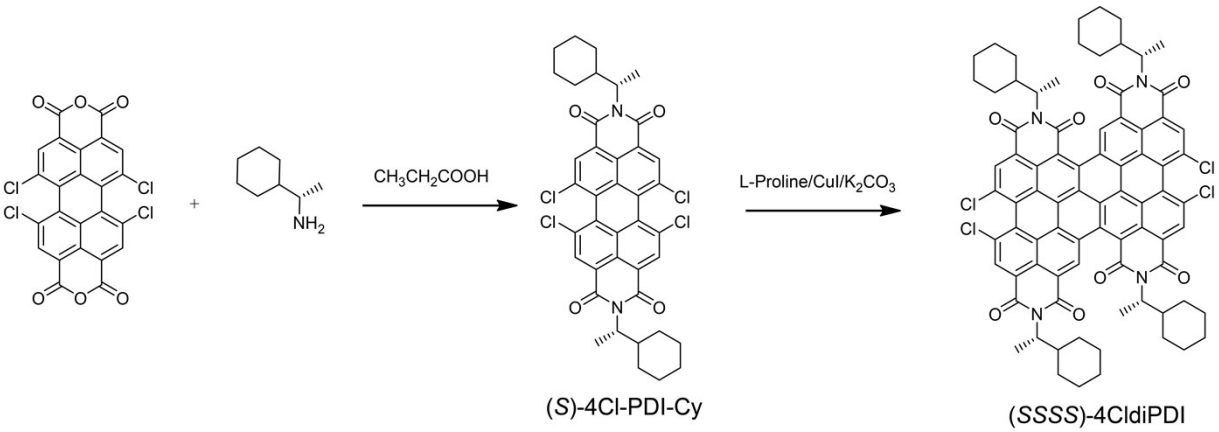
Computational Methods: The structures were optimized by using Density Functional Theory (DFT) with the PCM implicit solvation model in a DMF solution environment, employing the Gaussian 16 software[S2], the vibrational frequencies were calculated after geometries optimization and no imaginary frequency was found. The structure optimization and frequency analysis were obtained at the Becke three-parameter Lee-Yang-Parr (B3LYP) functional[S3] combining with 6-31G(d)[S4] basis set, and no imaginary frequency was found. Simulations of UV-vis and CD spectra, as well as electric and magnetic transition dipole moments, were performed using time-dependent DFT (TDDFT) calculations at the B3LYP/6-31G(d) level. Furthermore, the crystal structure optimization was carried out using the quantum mechanics/molecular mechanics (QM/MM) method within the ONIOM model, which was constructed based on X-ray crystal structures and implemented in a 3 × 3 × 3 supercell. In the QM/MM calculation, one innermost molecule was treated as a high-layer by an accurate high-level quantum mechanics method and the surrounding molecules were treated as a low-layer by the efficient universal force field (UFF) with charge equilibrium method, and the QM part was allowed to move while those in the MM part was frozen. Following geometry optimization, vibrational frequencies were calculated, with no imaginary frequency found. The absorption and circular dichroism spectra, along with the electric and magnetic transition dipole moments, were carried out through TD-DFT method based on the optimized S_0 geometry, the lowest 60 states were taken into consideration. For all of the aforementioned DFT calculations, the B3LYP functional was used in conjunction with a 6-31G(d) basis set.

Conformational searches were performed using Confab[S5] to generate one thousand distinct conformations for each molecule. Subsequently, the xtb software[S6], employing the GFN2-xTB semi-empirical method, was utilized to calculate the energies of these conformations.

To calculate the energy of the crystals, calculations were performed using DFT within the Vienna Ab initio Simulation Package (VASP, Version 5.4.4)[S7-S8], employing the Projector Augmented-Wave (PAW)[S9] method for implementation. The exchange-correlation functional

employed was the Perdew-Burke-Ernzerhof (PBE)[S10] Generalized Gradient Approximation (GGA). Van der Waals (vdW) dispersion corrections were implemented using Grimme's DFT-D3 method with zero-damping function. The plane-wave cutoff energy is set to 500 eV. All structures undergo relaxation until the convergence of energy and total forces are attained at thresholds of 10^{-5} eV and 0.05 eV $Å^{-1}$, respectively. The Γ-centered Monkhorst-Pack mesh k points with k-spacing of 0.04 π $Å^{-1}$ are utilized for Brillouin zone sampling.

2. NMR of Synthesized (*SSSS*)-, (*RRRR*)- and (*Rac*)-4CldiPDI



(*SSSS*)-4CldiPDI: (black solid, yield: 20%). ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 383K): δ 10.07 (d, *J* = 5.2 Hz, 2 H), 9.27 (s, 2 H), 9.04 (s, 2 H), 5.25 (td, *J* = 16.4, 8.4 Hz, 2 H), 5.12 (td, *J* = 14.4, 6.8 Hz, 2 H), 2.81−1.83 (m, 26 H), 1.72 (s, 12 H), 1.41−1.12 (m, 18 H). ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K): 163.0, 135.4, 135.2, 133.5, 131.2, 130.1, 129.1, 128.4, 128.2, 126.5, 126.3, 125.2, 124.9, 124.8, 124.0, 123.8, 123.2, 122.8, 121.5, 121.4, 119.6, 55.5, 54.9, 40.6, 38.7, 34.3, 30.9, 30.8, 30.6, 29.7, 29.2, 25.7, 25.6, 25.3, 22.2, 16.9, 16.2, 15.7, 13.8. HRMS (MALDI−TOF): calculated m/z for $[C80H66Cl4N4O8]^{-}$: 1350.3635; found: 1350.3617.

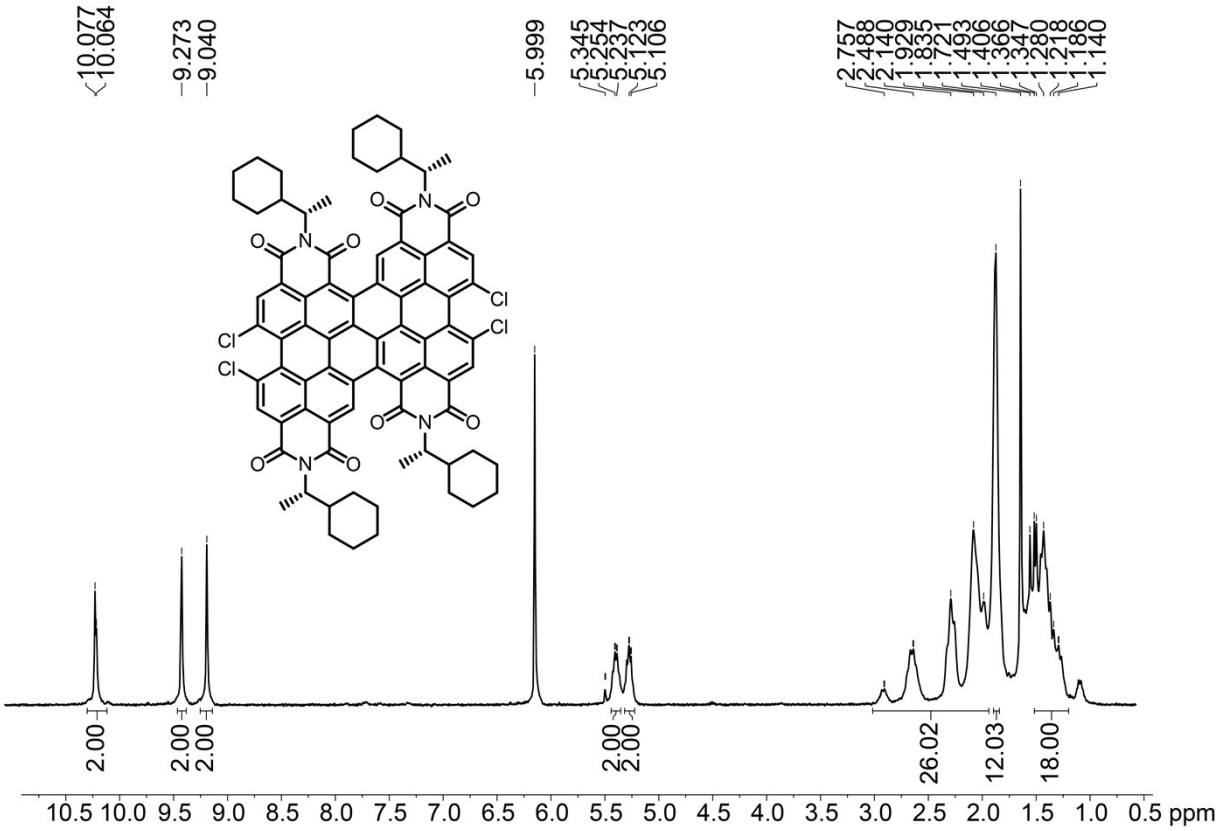


Figure S1. ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$, 383K) recorded for (*SSSS*)-4CldiPDI.

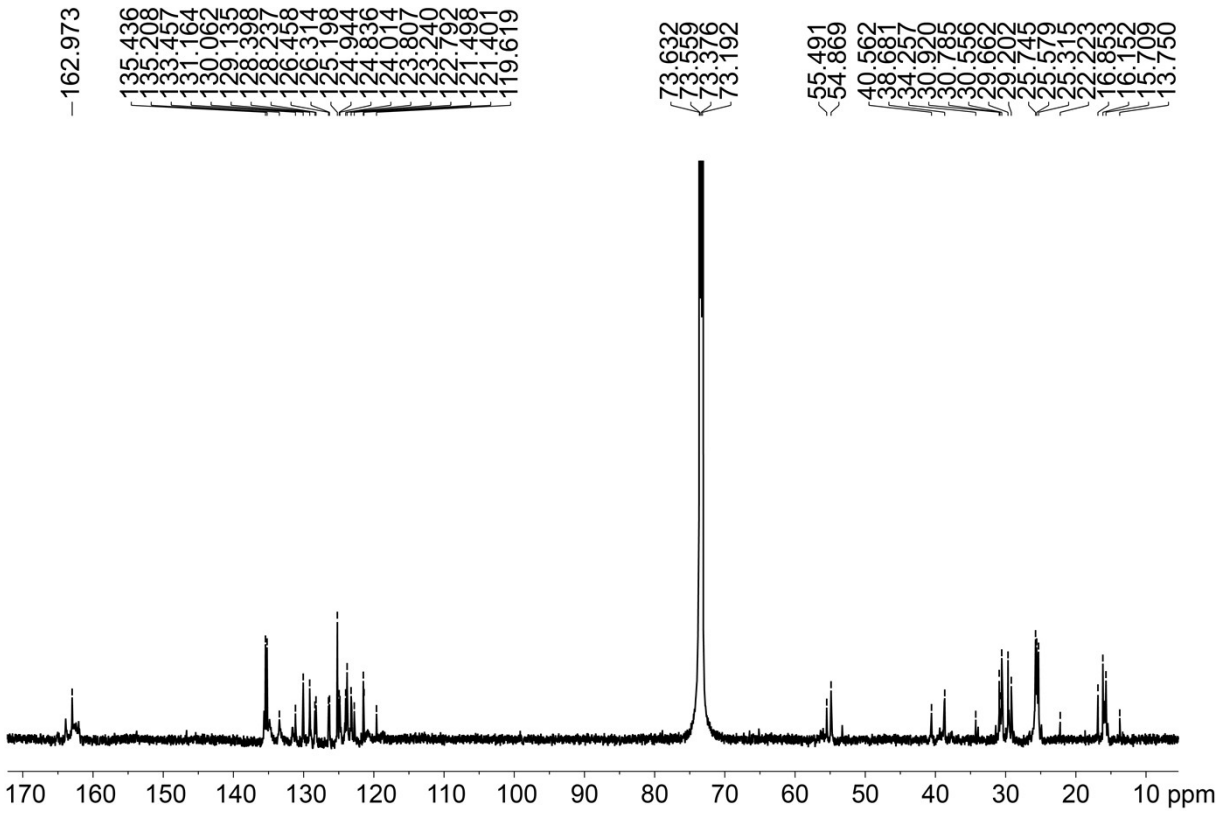
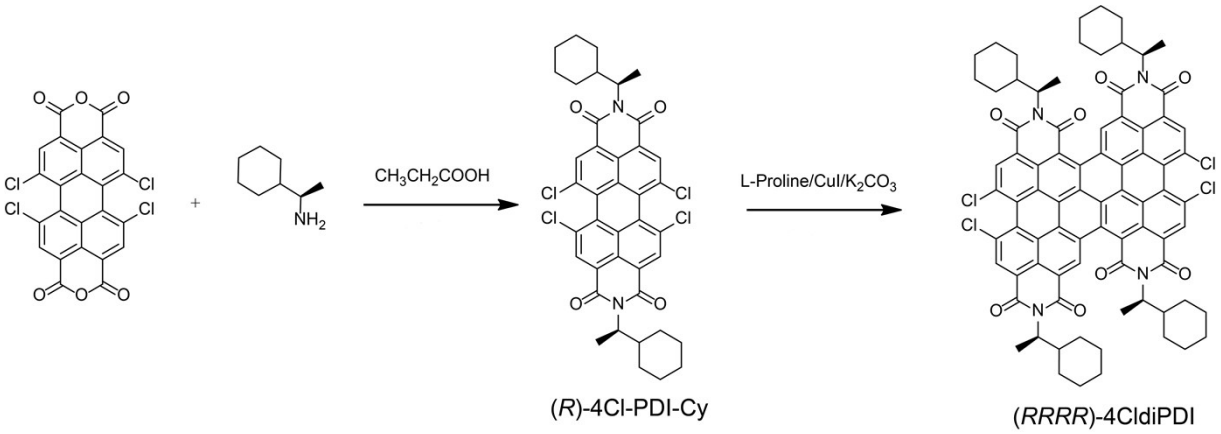


Figure S2. ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K) recorded for (*SSSS*)-4CldiPDI.



(*RRRR*)-4CldiPDI: (black solid, yield: 18%). ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 383K): δ 10.07 (d, *J* = 6.0 Hz, 2 H), 9.28 (d, *J* = 3.2 Hz, 2 H), 9.04 (s, 2 H), 5.25 (td, *J* = 16.0, 6.8 Hz, 2 H), 5.12 (td, *J* = 13.6, 6.8 Hz, 2 H), 2.81−1.83 (m, 26 H), 1.74−1.72 (m, 12 H), 1.42−1.12 (m, 18 H). ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K): 163.9, 163.0, 135.4, 135.2, 133.4, 131.2, 130.1, 129.1, 128.4, 128.2, 126.5, 126.3, 125.2, 124.9, 124.8, 124.0, 123.8, 123.2, 122.8, 121.5, 121.4, 119.8, 119.6, 55.5, 54.9, 40.6, 38.7, 31.1, 30.6, 25.7, 25.6, 25.3, 22.2, 22.1, 16.9, 16.1, 15.7, 13.7. HRMS (MALDI−TOF): calculated m/z for $[C80H66Cl4N4O8]^{-}$: 1350.3635; found: 1350.3622.

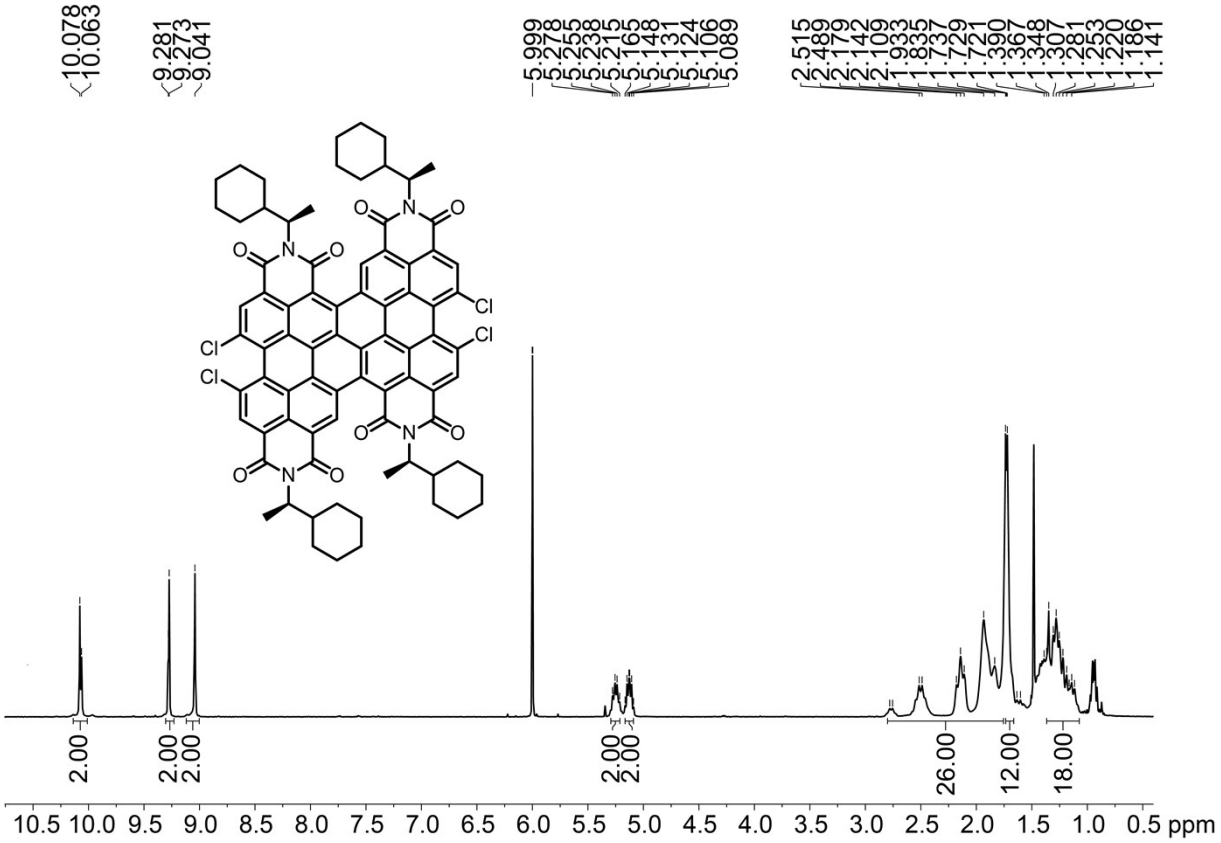


Figure S3. ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$, 383K) recorded for (*RRRR*)-4CldiPDI.

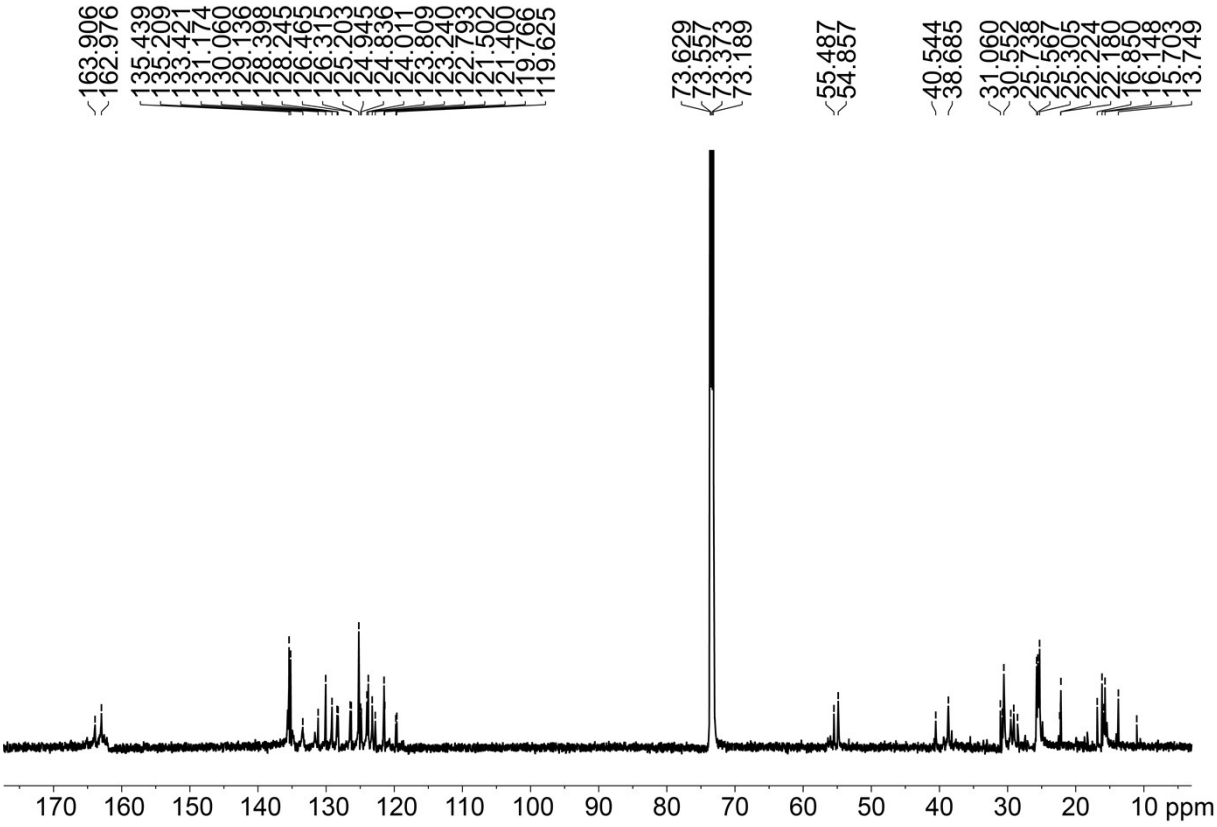
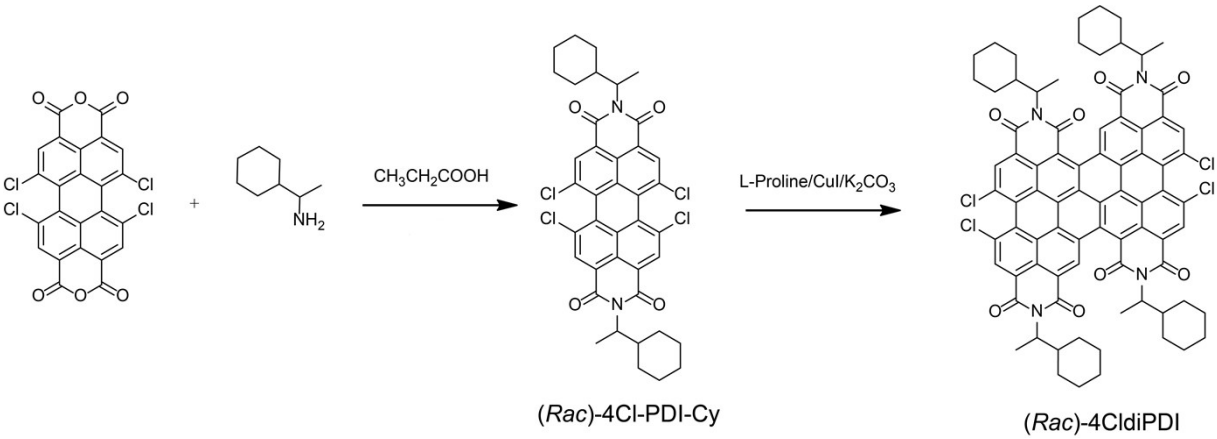


Figure S4. ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K) recorded for (*RRRR*)-4CldiPDI.



(*Rac*)-4CldiPDI: (black solid, yield: 16%). ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 383K): δ 10.07 (d, *J* = 6.0 Hz, 2 H), 9.28 (d, *J* = 3.2 Hz, 2 H), 9.04 (s, 2 H), 5.25 (td, *J* = 17.6, 5.2 Hz, 2 H), 5.13 (td, *J* = 16.8, 8.8 Hz, 2 H), 2.79−1.84 (m, 26 H), 1.75−1.71 (m, 12 H), 1.28−1.12 (m, 18 H). ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K): 166.0, 164.9, 137.4, 137.3, 137.1, 137.0, 132.0, 131.9, 131.4, 131.1, 130.3, 129.6, 128.6, 128.3, 128.2, 127.2, 126.9, 125.27 125.1, 124.6, 123.4, 123.3, 121.7, 57.5, 56.3, 42.4, 40.7, 37.2, 33.2, 32.3, 31.1, 31.0, 30.7, 27.2, 24.1, 18.1, 17.9, 15.7. HRMS (MALDI−TOF): calculated m/z for $[C80H66Cl4N4O8]^-$: 1350.3635; found: 1350.3629.

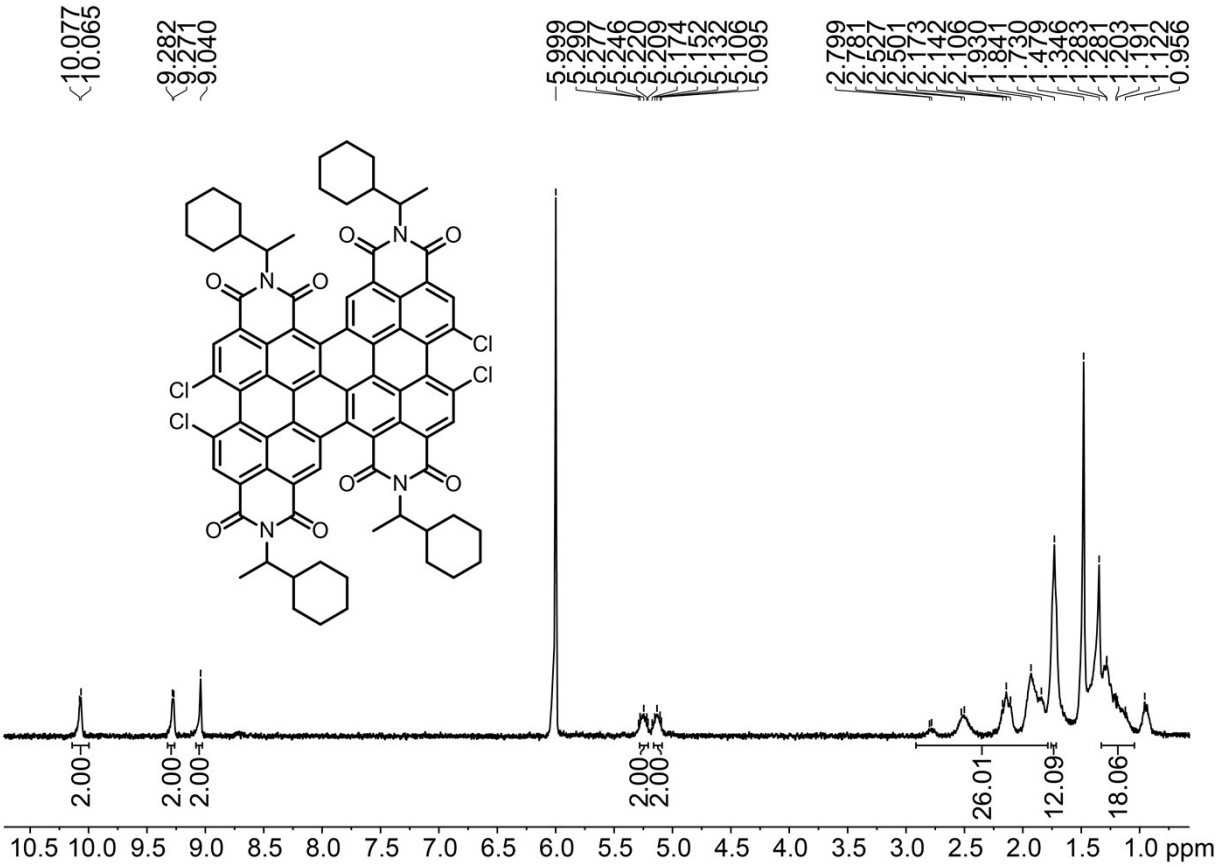


Figure S5. ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$, 383K) recorded for (*Rac*)-4CldiPDI.

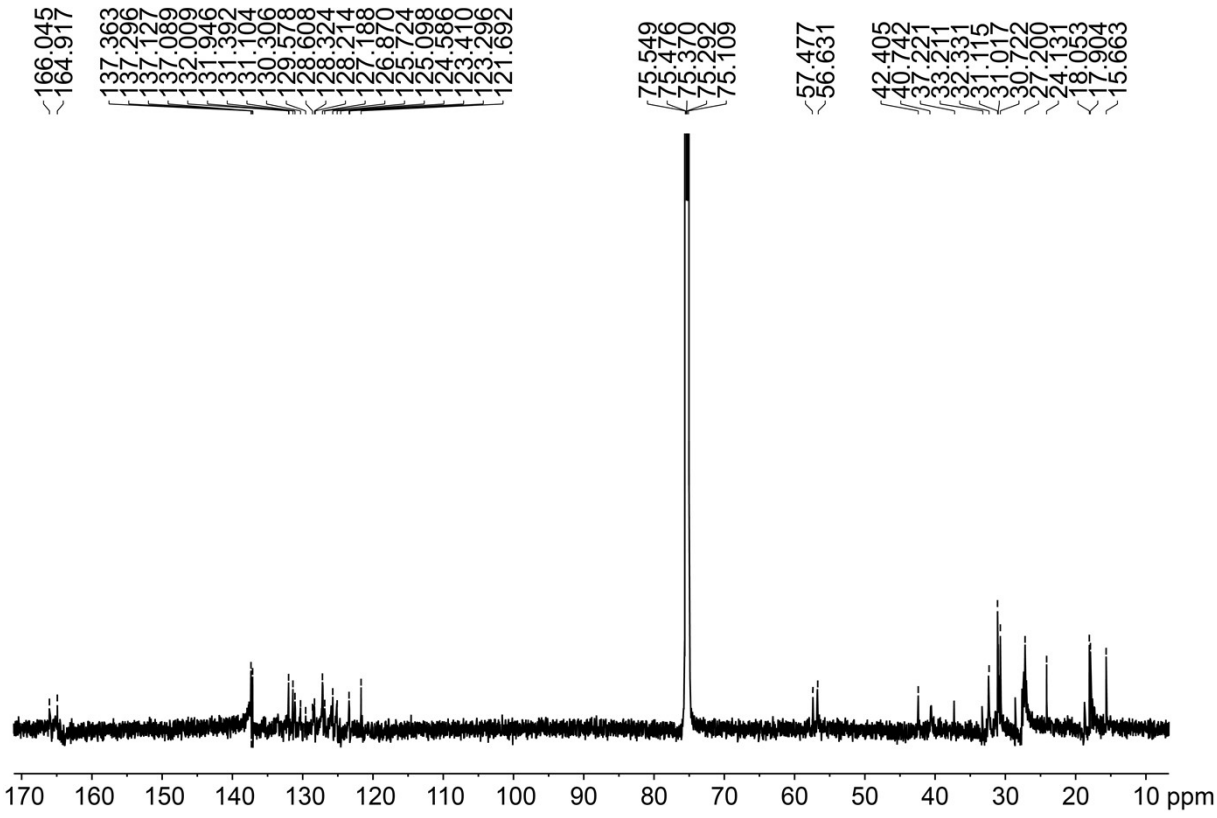


Figure S6. ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 298K) recorded for (*Rac*)-4CldiPDI.

3. Additional Figures

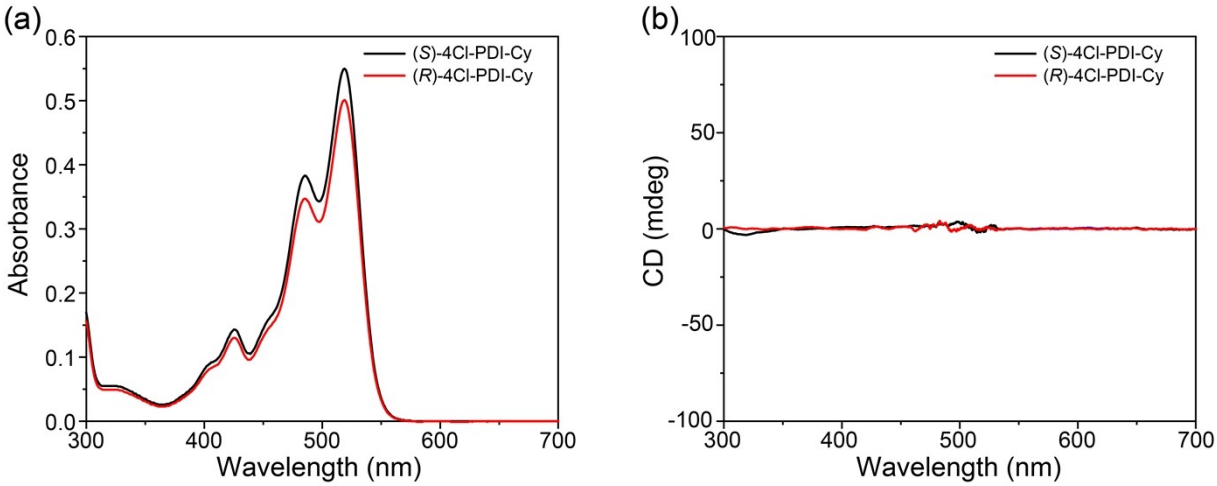


Figure S7. (a) UV-vis spectra and (b) CD spectra of (*S*)- and (*R*)-4Cl-PDI-Cy in DCM (10^{-5} M).

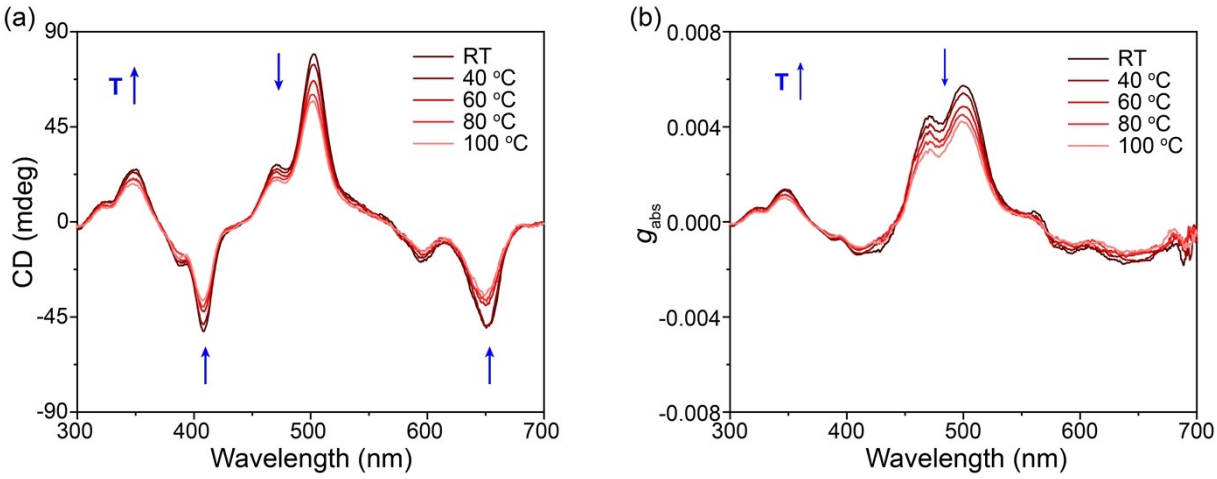


Figure S8. Variable-temperature CD of (*SSSS*)-4CldiPDI in tetrachloroethane solution (10^{-5} M).

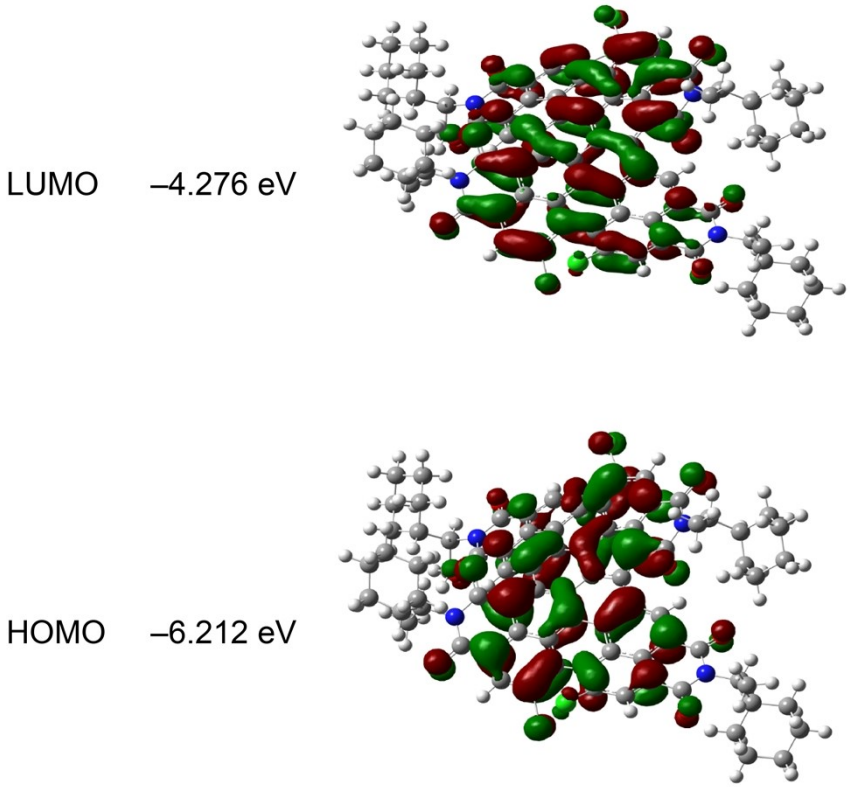


Figure S9. LUMO and HOMO electron distributions of (*SSSS*)-4CldiPDI obtained by DFT calculations.

4. X-ray Structure Determination

Data of (*SSSS*)-4CldiPDI was collected at 193.00 K on Bruker D8 VENTURE with Mo–Kα radiation (λ = 0.71073 Å) with a CCD area detector. All data were integrated with SAINT and a multi-scan absorption correction using SADABS was applied.[S11-S12] The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL using Olex2.[S13-S15] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. The guest molecules are severely disordered and therefore removed using Solvent Mask during structural refinement. Effective data standards (I/sigma above 3) were applied to the data refine process; thus the data was truncated by 1.25 (2 theta = 33 degrees). According to our calculations, there should be an extra 3 guest *N*,*N*-Dimethylformamide molecules per formula unit for (*SSSS*)-4CldiPDI. The crystal structure was used to confirm the connectivity, but a detailed geometrical analysis was not possible. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication on No. CCDC 2362311, the crystallographic data

were summarized below. Crystal data, data collection and structure refinement details are summarized in **Table S1**.

Table S1. Crystallographic data and refinement details for (*SSSS*)-4CldiPDI

	(*SSSS*)-4CldiPDI
CCDC	2362311
Moiety formula	$C_{80}H_{66}C_{l4}N_4O_8$, C_3H_7NO, 3[C_3H_7O]
Sum formula	$C_{92}H_{94}C_{l4}N_5O_{12}$
M_r	163.52
Temperature/K	193K
Crystal system	monoclinic
Space group	*P* 1
a/Å	14.924(3)
b/Å	15.705(3)
c/Å	17.535(4)
α/°	89.652(13)
β/°	88.476(13)
γ/°	78.232(12)
Volume/Å^3	4022.1(14)
Z	2
ρ_{calc} [gcm^{-3}]	1.324
μ [mm^{-1}]	0.215
F(000)	1690
Crystal size [mm^3]	0.18 × 0.15 × 0.13
Crystal colour	white
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	2.32 to 33.00 (1.25 Å)
Reflections collected	17960
Independent reflections	7006 R_{int} = 0.1240 R_{sigma} = 0.1712
Completeness to θ = 16.500°	99.5 %
Data / Restraints / Parameters	7006/5202/1831
Absorption correction	0.4212/0.7518
T_{min}/T_{max} (method)	(multi-scan)
Goodness-of-fit on F^2	1.055

Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0924$; w$R_2 = 0.2346$
Final R indexes [all data]	$R_1 = 0.1209$; w$R_2 = 0.2646$
Largest peak/hole [eÅ^{-3}]	0.63/−0.39
Flack X parameter	−0.21(14)

5. Theoretical Studies

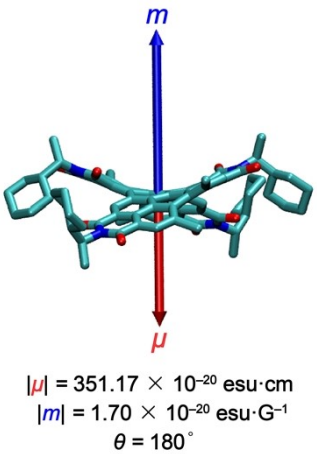


Figure S10. Electric (***μ*** is shown in red) and magnetic (***m*** is shown in blue) transition dipole moments for the $S_0 \rightarrow S_3$ transitions for the (*SSSS*)-4CldiPDI in monomers.

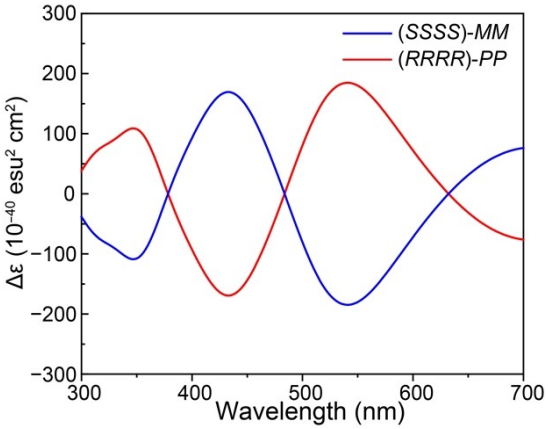


Figure S11. Simulated CD spectra of (*SSSS*)-*MM* and (*RRRR*)-*PP* conformers in the monomeric state.

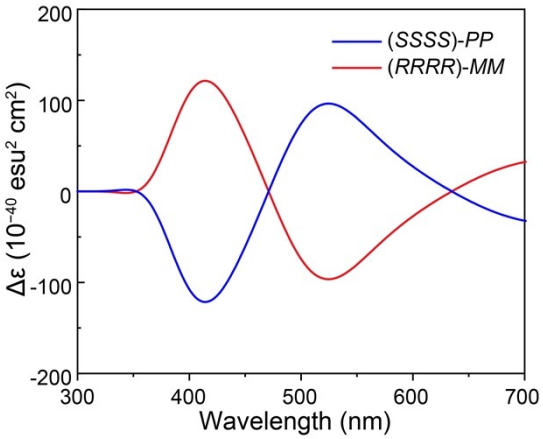


Figure S12. Simulated CD spectra of (*SSSS*)-*PP* and (*RRRR*)-*MM* in crystal based on quantum mechanics/molecular mechanics (QM/MM) method in the ONIOM model.

Table S2. Optimized geometry for (*SSSS*)-*PP* in the monomeric state.

(*SSSS*)-*PP*			
S_0 state			
b3lyp/6-31g(d)			
E = −5751.217670			
Cl	−2.67944216	6.29791048	1.65069914
Cl	2.67943215	−6.29784946	1.65050314
Cl	−2.12486912	6.52748249	−1.43291509
Cl	2.12481511	−6.52733548	−1.43309609
O	4.01693829	1.60936608	−1.89908012
O	−4.0169793	−1.60920109	−1.89904812
O	−3.02451726	−6.06807842	−2.09563913
O	6.41770848	0.72322201	1.45236612
O	−7.16441848	3.71020431	2.39504919
O	−6.41765149	−0.72316502	1.45258112
N	6.85888847	−1.48979116	1.89555215
O	7.16430751	−3.71010332	2.39514319
C	3.27552525	2.52687615	−1.56455409
C	−1.62624813	−0.97813207	−0.40434701
N	−6.85888551	1.48984715	1.89570715
N	−3.61941129	−3.86220326	−1.87974412
C	6.03753844	−0.44316908	1.42436312
C	4.70120233	−0.79776209	0.88345208
O	3.02442825	6.06824543	−2.09559314
N	3.61933528	3.86236125	−1.87979012
C	0.72476004	−1.72232214	−0.240549
C	−0.93613804	5.32645937	−0.97582505
C	−0.32015901	3.06585222	−0.42202001
C	2.10743814	−1.41495612	−0.00855598
C	0.22662602	0.68188504	−0.273801
C	1.01222509	3.30081122	−0.86834405
C	−0.22664302	−0.68176605	−0.273805

C	6.44370442	−2.82648425	1.94585316
C	3.87126027	0.20207998	0.43247405
H	4.21935131	1.22147106	0.50791105
C	2.9829052	−2.4780612	0.37641104
C	−0.72478204	1.72243812	−0.240501
C	−2.56207518	0.08069602	−0.03805899
C	2.56206618	−0.08058903	−0.03814999
C	1.34632912	4.59375731	−1.33365508
C	1.98194316	2.26920214	−0.86311304
C	−2.10745215	1.41506611	−0.00846998
C	2.71723522	4.92143333	−1.78861211
C	−3.27558525	−2.52672317	−1.5645031
C	−6.03749246	0.44323306	1.42459612
C	−6.44374744	2.82656624	1.94591215
C	0.37077106	5.56570638	−1.42995509
H	0.62244908	6.52241546	−1.87154612
C	−3.87124528	−0.201992	0.43261705
H	−4.21930132	−1.22139107	0.50809605
C	2.53584015	−3.8394663	0.36935604
C	−2.71730823	−4.92127734	−1.78863311
C	−1.98198916	−2.26907116	−0.86308505
C	1.62622812	0.97825305	−0.40438601
C	−0.37083406	−5.56556441	−1.43005208
H	−0.62252209	−6.52225845	−1.87167012
C	1.27587107	−4.13275131	−0.32259501
C	0.320122	−3.06573323	−0.42207401
C	0.93608803	−5.32632538	−0.97595505
C	−1.0122751	−3.30068324	−0.86836504
C	−2.53585916	3.83956728	0.36948304
C	5.08560634	−3.14492727	1.43323412
C	−1.34639213	−4.59362033	−1.33369608
C	−8.20589657	1.08926812	2.43428519
C	−9.39615966	1.37101215	1.47567712
H	−10.22089171	0.80312811	1.93784915
C	−4.2679373	2.14783818	0.87425308
C	−10.95625277	2.29810823	−0.89247305
H	−11.89091182	2.32759224	−1.46741209
H	−10.2274597	2.90874227	−1.44611609
C	−3.30964021	4.75345235	1.1107301
C	−4.97874339	−4.07759927	−2.49293217
C	4.26792929	−2.14775319	0.87412908
C	−4.5832223	4.42480434	1.59309213
H	−5.17178934	5.1658444	2.12026317
C	6.02333046	4.72306529	−1.54032209
H	6.97447555	4.53937328	−2.06763813
C	3.30961321	−4.75336337	1.1105891
C	4.97864638	4.07775926	−2.49301916
C	−6.02335649	−4.72291031	−1.54020409
H	−6.97455355	−4.53912829	−2.06739013

C	8.20590958	−1.08923514	2.43412419
C	−9.17151365	0.76665411	0.07426402
H	−8.35433158	1.30732414	−0.42552801
H	−8.84849364	−0.27768897	0.16204003
C	9.39620564	−1.37132516	1.47566112
H	10.22088372	−0.80316913	1.93760316
C	−5.08563035	3.14500625	1.43334212
C	−2.9829182	2.47816019	0.37652604
C	−4.70118534	0.79784008	0.88362008
C	−7.25451657	−5.99824237	0.85876908
H	−6.38214348	−6.25385843	1.47864712
H	−8.14129963	−6.33420844	1.41182012
C	−1.27590407	4.1328693	−0.32248301
C	4.5831853	−4.42471936	1.59298413
H	5.17173334	−5.16575541	2.12017817
C	−8.4214556	1.54927716	3.8817823
H	−7.56946652	1.25417513	4.50415834
H	−8.56082861	2.62533423	3.9745753
H	−9.31106769	1.04406512	4.27451633
C	−7.29924258	−4.47745428	0.65310706
H	−8.23794163	−4.20902126	0.14599003
H	−7.30830453	−3.95915625	1.62029013
C	−6.11364747	−3.98256725	−0.1911
H	−5.1823184	−4.14424227	0.37191204
H	−6.19996247	−2.90120618	−0.35166901
C	9.17154667	−0.76759112	0.07398002
H	8.35444958	−1.30857216	−0.42561101
H	8.84839961	0.27675496	0.16129503
C	11.16557778	−2.90725729	0.50239105
H	11.49063379	−3.95224236	0.41652505
H	11.97722084	−2.36878725	1.01454009
C	10.43630173	−0.85790914	−0.79519704
H	11.2189798	−0.21974709	−0.35880501
H	10.23024974	−0.4580411	−1.79645211
C	6.11379648	3.98259724	−0.191301
H	5.1825104	4.14416126	0.37181804
H	6.20016244	2.90126216	−0.35197501
C	−10.43621775	0.85674512	−0.79501104
H	−10.23016475	0.45641009	−1.79608011
H	−11.21899383	0.21886708	−0.35837801
C	4.89736138	4.7111653	−3.88734026
H	5.89205444	4.66869229	−4.34513029
H	4.21299533	4.13944526	−4.52381331
H	4.56694936	5.7489684	−3.86724626
C	−4.89747538	−4.71097032	−3.88727626
H	−5.89217345	−4.66849531	−4.34505329
H	−4.56704637	−5.74876737	−3.86722526
H	−4.21312733	−4.13921328	−4.52373431
C	−11.16531679	2.90673127	0.50165005

H	−11.49024183	3.95171935	0.41532605
H	−11.97705484	2.36857524	1.01398109
C	−7.14933958	−6.73536744	−0.48429602
H	−8.07393564	−6.57456043	−1.05907806
H	−7.06990758	−7.81767055	−0.31867601
C	8.42129758	−1.54892417	3.8817443
H	9.31104864	−1.04387814	4.27437533
H	7.56937656	−1.25340615	4.50401234
H	8.56035362	−2.62500025	3.9748193
C	7.25464955	5.99824835	0.85864708
H	8.1414596	6.33422241	1.41164912
H	6.38231351	6.25377741	1.47861213
C	7.14932958	6.73547042	−0.48435502
H	7.06987853	7.81775849	−0.31864901
H	8.07387864	6.57473241	−1.05923206
C	5.94513647	6.2445194	−1.30606408
H	5.0194664	6.49203941	−0.77500404
H	5.90510247	6.77807543	−2.26261214
C	−9.8854887	2.82751526	1.35136912
H	−10.06961068	3.25654329	2.34273418
H	−9.10639966	3.4432123	0.88741808
C	9.88568767	−2.82783227	1.35199411
H	10.06979071	−3.25642831	2.34355419
H	9.10669865	−3.44380831	0.88825708
C	10.95651477	−2.29925524	−0.89200405
H	10.22782272	−2.91021628	−1.44541909
H	11.89120483	−2.32887525	−1.46688509
C	−5.94520849	−6.2443934	−1.30608207
H	−5.01949241	−6.49198343	−0.77513104
H	−5.90528747	−6.77787244	−2.26267215
C	7.29943457	4.47748327	0.65285806
H	7.30859155	3.95910823	1.61999414
H	8.23811261	4.20913924	0.14564803
H	−5.32461143	−3.05566919	−2.63788917
H	−8.12106358	0.00366604	2.4639852
H	8.12119556	−0.00361706	2.46355619
H	5.3245084	3.05582818	−2.63798817

Table S3. Optimized geometry for (*RRRR*)-*MM* in the monomeric state.

Cl	2.679544	6.297875	1.650576
Cl	−2.679555	−6.297798	1.650614
Cl	2.124935	6.527406	−1.433032
Cl	−2.124931	−6.527355	−1.43296
O	−4.016912	1.60936	−1.899106
O	4.01692	−1.609308	−1.899054
O	3.024369	−6.068152	−2.095685
O	−6.417716	0.723319	1.452339
O	7.164496	3.710117	2.394903

O	6.417633	−0.723257	1.452548
N	−6.858942	−1.489678	1.895552
O	−7.164469	−3.710006	2.395008
C	−3.275521	2.526871	−1.56453
C	1.626221	−0.978185	−0.404348
N	6.858921	1.48976	1.895597
N	3.619333	−3.862307	−1.879697
C	−6.037557	−0.443078	1.424388
C	−4.701227	−0.797699	0.883477
O	−3.024371	6.068208	−2.095734
N	−3.619324	3.86236	−1.879762
C	−0.724799	−1.722338	−0.240514
C	0.936189	5.32641	−0.975915
C	0.320187	3.065822	−0.42206
C	−2.107471	−1.414948	−0.008519
C	−0.226626	0.681863	−0.2738
C	−1.0122	3.300792	−0.868373
C	0.226621	−0.681797	−0.27379
C	−6.443798	−2.826388	1.945826
C	−3.871267	0.202125	0.432492
H	−4.219335	1.221522	0.507923
C	−2.982957	−2.478033	0.376456
C	0.724795	1.722403	−0.240527
C	2.562068	0.08064	−0.038097
C	−2.562076	−0.080573	−0.038125
C	−1.346292	4.593734	−1.333708
C	−1.981931	2.269195	−0.863112
C	2.107465	1.415016	−0.008516
C	−2.717193	4.921408	−1.788686
C	3.275527	−2.526816	−1.564475
C	6.037519	0.443153	1.424482
C	6.443804	2.826485	1.945784
C	−0.37072	5.565667	−1.430036
H	−0.622384	6.522362	−1.871663
C	3.871249	−0.202057	0.432546
H	4.219306	−1.221456	0.508009
C	−2.535913	−3.839445	0.369425
C	2.717199	−4.921354	−1.788623
C	1.981933	−2.269135	−0.863068
C	−1.626225	0.978249	−0.404376
C	0.370724	−5.565612	−1.429977
H	0.622391	−6.522312	−1.871592
C	−1.275947	−4.132761	−0.322517
C	−0.320188	−3.065758	−0.422029
C	−0.936185	−5.326353	−0.975859
C	1.012201	−3.300732	−0.868331
C	2.53591	3.839517	0.369394
C	−5.085689	−3.144853	1.433249
C	1.346296	−4.593677	−1.333654

C	8.205926	1.089174	2.434186
C	9.396201	1.37099	1.475614
H	10.220878	0.802916	1.937652
C	4.267973	2.147773	0.874158
C	10.956359	2.298411	−0.892363
H	11.891011	2.327911	−1.467313
H	10.227625	2.909243	−1.445863
C	3.30971	4.753401	1.110618
C	4.978668	−4.077733	−2.492866
C	−4.267983	−2.147697	0.874155
C	4.583295	4.424744	1.592969
H	5.171875	5.165781	2.120128
C	−6.023201	4.723232	−1.540176
H	−6.974406	4.539644	−2.06742
C	−3.309713	−4.75332	1.110657
C	−4.978657	4.077793	−2.492925
C	6.023225	−4.723179	−1.540133
H	6.974417	−4.539634	−2.067418
C	−8.205974	−1.089092	2.434077
C	9.171465	0.766952	0.074077
H	8.354338	1.307822	−0.425586
H	8.848328	−0.277374	0.161638
C	−9.396242	−1.371184	1.475577
H	−10.220936	−0.80303	1.937484
C	5.085687	3.144938	1.433225
C	2.982951	2.478105	0.376448
C	4.701209	0.797772	0.88352
C	7.254285	−5.998489	0.858897
H	6.381898	−6.253867	1.478851
H	8.141032	−6.334586	1.411926
C	1.275948	4.132825	−0.322557
C	−4.583295	−4.424655	1.593012
H	−5.171872	−5.165683	2.120188
C	8.421437	1.549115	3.88171
H	7.569455	1.253929	4.504056
H	8.560743	2.625177	3.97456
H	9.311072	1.043937	4.274431
C	7.299308	−4.477736	0.65307
H	8.238035	−4.209548	0.145871
H	7.308528	−3.95934	1.620193
C	6.113758	−3.982699	−0.191126
H	5.182438	−4.144118	0.371976
H	6.200286	−2.90138	−0.351828
C	−9.171536	−0.767472	0.073897
H	−8.354401	−1.308437	−0.425649
H	−8.848425	0.276884	0.161209
C	−11.165528	−2.907185	0.50224
H	−11.490543	−3.952182	0.416381
H	−11.977219	−2.368731	1.014328

C	−10.436248	−0.857841	−0.795338
H	−11.218968	−0.219701	−0.358991
H	−10.230159	−0.457974	−1.796586
C	−6.11365	3.982787	−0.191145
H	−5.182308	4.144249	0.371909
H	−6.200154	2.90146	−0.351813
C	10.436166	0.857084	−0.795196
H	10.230052	0.456984	−1.796345
H	11.218877	0.219028	−0.358708
C	−4.897428	4.711118	−3.887289
H	−5.892159	4.668707	−4.344998
H	−4.213161	4.139307	−4.523787
H	−4.566921	5.748891	−3.867275
C	4.897437	−4.711033	−3.887241
H	5.89217	−4.668618	−4.344948
H	4.566926	−5.748806	−3.867246
H	4.213174	−4.139205	−4.523727
C	11.165515	2.906715	0.501885
H	11.490555	3.951683	0.415777
H	11.9772	2.368361	1.014089
C	7.148884	−6.73573	−0.484088
H	8.073474	−6.575155	−1.058943
H	7.069258	−7.817999	−0.318351
C	−8.421413	−1.548767	3.881695
H	−9.311144	−1.043674	4.27431
H	−7.569487	−1.253296	4.503981
H	−8.560523	−2.624835	3.974761
C	−7.25418	5.998569	0.858882
H	−8.14091	6.334656	1.411944
H	−6.381771	6.253982	1.478792
C	−7.148857	6.735783	−0.484124
H	−7.069244	7.818058	−0.318414
H	−8.073471	6.575178	−1.058932
C	−5.944795	6.244678	−1.305937
H	−5.019045	6.492084	−0.774965
H	−5.904786	6.778222	−2.262492
C	9.885692	2.827464	1.351608
H	10.069882	3.256256	2.343062
H	9.106665	3.44335	0.887806
C	−9.885692	−2.827702	1.351923
H	−10.069857	−3.25626	2.343484
H	−9.106655	−3.443677	0.888258
C	−10.956406	−2.299204	−0.892155
H	−10.227664	−2.910149	−1.44552
H	−11.891064	−2.328863	−1.467086
C	5.944793	−6.244618	−1.305853
H	5.019064	−6.491992	−0.774831
H	5.904727	−6.778184	−2.262395
C	−7.299175	4.47781	0.653092

H	−7.30834	3.959432	1.620226
H	−8.237917	4.209587	0.145939
H	5.324602	−3.055811	−2.637739
H	8.121107	0.003568	2.463828
H	−8.121241	−0.003475	2.463501
H	−5.324598	3.055876	−2.637808

Table S4. Optimized geometry for (*SSSS*)-*MM* in the crystal state.

Cl	9.47138	4.34298	16.28535
Cl	7.39683	11.05829	10.51384
Cl	10.85966	4.17607	1.66296
Cl	6.58128	3.34835	16.52131
Cl	9.30199	11.03942	7.6838
Cl	4.4691	11.70336	9.82207
Cl	13.74179	3.44447	0.87502
Cl	12.20129	12.02046	7.72951
O	4.2302	3.86388	6.39729
O	14.12594	4.5296	10.6168
O	4.2734	10.72811	2.05683
O	9.39251	6.25807	5.36122
O	10.79551	8.94355	4.00526
O	3.99869	14.1178	5.16232
O	7.40455	3.20315	9.3237
O	9.16889	9.137	14.02305
O	8.22513	12.07418	17.45621
O	14.43733	11.39176	15.10258
O	14.74644	1.19798	13.73008
O	10.95231	12.0265	0.58991
O	7.94189	6.28321	12.70608
O	12.86577	14.68293	12.27885
O	5.85961	0.60445	3.57111
O	10.52105	3.28583	8.70874
O	3.78276	6.12315	1.02361
O	1.65244	4.86069	13.51794
N	13.68431	13.08795	13.74675
N	7.79399	4.72131	11.00654
N	14.46626	2.84329	12.12709
N	10.71762	10.49798	2.29306
N	8.66696	10.6452	15.70259
N	4.10518	12.45092	3.56068
N	5.04288	2.16837	5.07224
N	9.99901	4.73115	6.9915
N	1.78246	5.62638	15.69525
N	2.81639	5.71105	3.07632
C	4.97107	3.51759	5.46846
C	6.00808	9.21046	3.74776
C	12.02957	8.75049	11.65258
C	12.67403	6.77138	14.77001
C	7.36357	4.37298	9.71724

C	6.85554	5.44459	8.84729
C	12.33709	8.45059	12.99795
C	13.93102	4.08781	11.75377
C	5.97605	8.48815	6.09448
C	11.55843	8.44022	0.4995
C	6.42278	3.65485	0.65412
C	14.0396	2.96733	15.81283
C	10.72115	6.91699	8.67072
C	6.56657	5.21128	2.47489
C	6.1169	7.44878	7.05618
C	6.28349	6.83273	4.29301
C	13.18449	4.86556	12.77023
C	10.07477	7.16153	7.44553
C	13.88855	3.27939	14.47503
C	10.89166	5.58301	9.11699
C	12.4878	7.09133	13.40837
C	6.09368	4.20427	3.36763
C	6.12545	8.1854	4.7231
C	7.69492	6.0268	11.5279
C	6.51009	5.108	7.5611
C	12.39527	7.43195	17.11071
C	6.35699	7.80789	8.41428
C	6.54551	6.54863	2.93406
C	9.78372	6.03791	6.51047
C	6.52487	8.95288	2.42753
C	12.6081	9.48818	13.93236
C	6.1523	6.10147	6.63209
C	5.93531	2.88025	2.9034
C	12.44174	6.05353	17.5131
C	5.77523	4.5031	4.70997
C	11.03559	10.85508	0.97178
C	11.16572	7.99738	9.47899
C	12.541	9.15639	15.33885
C	6.75918	7.62084	2.02007
C	9.72211	8.46828	7.12768
C	12.58107	7.8029	15.74666
C	5.63263	1.78174	3.85581
C	10.88171	9.19336	2.80312
C	13.05827	13.49783	12.55917
C	4.57614	11.18453	3.16537
C	8.3013	10.91574	17.03741
C	8.85759	9.34393	15.19857
C	13.32291	4.52608	14.13092
C	14.39179	2.3413	13.4327
C	12.87931	10.77192	13.41873
C	6.06491	2.6292	1.54883
C	6.91732	10.01145	1.58758
C	11.99548	10.09222	11.20875
C	12.02094	11.67609	9.40534

C	6.29838	9.17924	8.83705
C	4.26311	12.95127	4.86447
C	11.74992	7.69155	10.74157
C	12.55188	6.07315	12.41933
C	11.18069	8.11626	1.81558
C	5.37304	10.40676	4.13769
C	6.0459	5.78517	5.22518
C	4.59508	12.26088	7.23674
C	5.69724	10.15109	7.90938
C	5.70626	9.8129	6.51373
C	14.44147	14.02806	14.63821
C	15.0634	15.20434	13.90647
C	13.64131	3.86175	16.82652
C	5.01589	11.3486	8.22668
C	13.71393	11.74142	14.1637
C	12.35176	15.19448	15.65405
C	5.27667	10.73186	5.50758
C	7.4369	5.98421	0.28067
C	11.4852	9.78715	0.06529
C	7.26661	7.10344	10.5851
C	4.72815	11.97731	5.88799
C	12.22761	10.14246	16.2921
C	11.60793	10.40599	9.86279
C	8.56771	11.84845	14.81912
C	9.48717	11.8498	13.60532
C	11.98176	6.35348	11.12702
C	7.05756	12.14229	14.57947
C	11.53633	3.2073	5.79691
C	8.0921	8.44031	17.41706
C	10.36299	11.66826	3.15476
C	9.40788	11.33995	4.29156
C	4.41022	12.44813	13.2816
C	8.68778	5.83684	16.64094
C	3.38516	13.20061	2.47582
C	17.23138	14.13605	2.99904
C	6.79782	6.78543	9.29696
C	8.97509	6.91256	15.78217
C	5.19535	0.91988	7.25235
C	6.94387	9.45657	10.06759
C	10.04197	3.52652	6.10524
C	9.08801	3.5448	4.92107
C	10.96469	9.35559	9.07024
C	4.34317	1.2097	5.99735
C	6.95584	15.36797	5.30642
C	11.38259	5.76508	1.24246
C	4.39768	13.84318	1.49147
C	11.04615	6.77705	2.16233
C	8.18715	3.53886	11.83656
C	9.21083	3.83036	12.92245

C	6.15058	10.93269	14.30423
C	10.0914	9.53296	7.96806
C	6.90432	2.79436	12.28621
C	8.64355	8.21264	16.14304
C	7.25663	7.33612	0.71719
C	10.44309	4.44767	8.2998
C	13.61813	14.36693	15.89723
C	12.66908	12.4117	11.62562
C	11.51457	5.30872	10.30954
C	7.46621	9.75692	0.35412
C	12.51886	11.08633	12.08936
C	2.5796	0.68149	0.06543
C	6.86235	4.91929	1.10258
C	14.03603	2.99685	4.2175
C	12.45309	12.68408	10.28697
C	13.1171	0.61792	10.70632
C	13.1054	1.79315	4.36507
C	7.38179	8.44152	10.94188
C	11.36376	13.63121	4.45464
C	6.48258	15.23948	1.15252
C	11.65047	12.45186	3.51948
C	5.47719	14.69059	2.16805
C	5.79857	3.65746	12.90682
C	11.65849	2.18527	4.6645
C	15.18208	2.14037	11.00789
C	1.35668	1.19138	11.46315
C	13.8909	3.973	5.38194
C	5.96058	0.74856	13.41414
C	4.52626	2.8189	13.06523
C	6.4682	0.10199	7.01387
C	12.43336	4.42301	5.51903
C	14.15323	1.5191	10.02847
C	4.68338	11.37747	14.33838
C	16.39665	5.73107	14.37927
C	5.38281	13.6259	13.38141
C	12.59564	14.53514	4.57948
C	12.08058	0.10124	9.70608
C	14.07512	12.51017	4.13541
C	5.15054	15.24127	16.91802
C	11.55982	15.35203	16.95707
C	14.49645	15.04627	16.96058
C	13.80039	0.253	7.86799
C	14.83583	0.77116	8.87201
C	9.61833	14.68192	9.42209
C	15.95309	14.74079	8.54313
C	5.1131	0.08447	9.64289
C	4.33079	0.25604	8.33876
C	6.84838	13.19832	13.49286
C	7.21466	1.60465	13.20027

C	4.76446	1.56771	13.91586
C	13.8514	13.75903	4.99557
C	3.68432	14.66684	0.40555
C	12.82498	11.62562	4.06033
C	10.46656	15.31922	8.31626
C	13.2578	15.20727	0.74161
C	8.74446	0.59991	0.53317
C	16.43397	6.70722	16.62655
C	3.44173	6.48895	2.15527
C	2.41196	6.23771	4.36788
C	2.42473	4.43007	16.21883
C	2.45088	4.34204	2.75376
C	12.93684	5.4373	15.1616
C	12.98202	5.07975	16.55116
H	14.52234	2.02756	16.08619
H	6.63072	4.0678	7.26721
H	9.69318	2.72496	6.7723
H	9.14988	8.66863	6.22163
H	5.85241	1.63292	1.16098
H	6.82869	11.04892	1.90335
H	4.11794	13.1935	7.54043
H	11.72344	14.72169	14.88288
H	9.42381	0.81307	15.25755
H	12.10409	11.18655	16.01345
H	6.6994	12.57746	15.5309
H	11.9339	2.73871	6.71556
H	3.37266	12.81482	13.35563
H	4.51151	11.97555	12.29156
H	9.46159	6.7285	14.8241
H	5.50658	1.90072	7.6564
H	15.66133	2.9748	10.47389
H	4.9101	13.00499	0.98319
H	10.6339	6.5154	3.14063
H	6.38922	10.4885	13.32178
H	6.3007	10.14168	15.05439
H	6.48247	2.37521	11.35655
H	13.29976	13.39963	16.32758
H	11.59648	4.26863	10.61696
H	2.12914	1.58577	0.51854
H	3.77278	1.04493	16.84419
H	15.27206	13.3968	14.9892
H	13.77551	3.54557	3.29778
H	15.07865	2.65494	4.10766
H	12.64929	13.68563	9.90389
H	12.60437	1.17144	11.50653
H	16.83005	15.13981	11.1905
H	9.81603	12.31936	2.45589
H	13.11524	1.20216	3.43906
H	13.48856	1.1356	5.16162

H	7.84894	8.7062	11.89409
H	10.50696	14.2197	4.09162
H	11.08983	13.24984	5.45324
H	8.9255	12.65659	15.4744
H	7.02429	14.39554	0.69062
H	4.03652	0.46711	1.67696
H	11.9915	12.88378	2.56183
H	1.79716	0.1525	2.71104
H	6.01084	14.09165	2.92096
H	6.12363	4.06345	13.88084
H	5.57327	4.53	12.27342
H	11.07413	1.28389	4.90457
H	11.21496	2.60881	3.75106
H	14.20797	3.48998	6.32439
H	14.54725	4.84679	5.23955
H	9.38914	15.30551	14.11881
H	5.69679	0.27238	12.45442
H	4.19233	2.51241	12.05762
H	3.7094	3.42974	13.47736
H	9.40687	14.48155	6.6157
H	7.09298	0.58324	6.2437
H	12.10993	4.93592	4.59514
H	12.36146	5.16091	6.33257
H	13.60406	2.36671	9.58033
H	4.01608	10.51306	14.19133
H	4.46148	11.77898	15.34446
H	3.49578	1.81418	6.35543
H	15.93507	6.71662	14.13643
H	2.88744	12.39191	1.91867
H	5.27345	14.27183	12.50127
H	5.11425	14.25077	14.24749
H	12.39288	15.33962	5.30703
H	12.77077	15.02804	3.60783
H	11.4978	0.95591	9.31971
H	14.56549	14.82429	10.2266
H	14.93234	11.93269	4.51996
H	14.34098	12.81971	3.10821
H	5.62418	14.40129	16.38148
H	1.42121	0.46222	16.1541
H	11.2166	14.35937	17.29065
H	7.45498	0.58139	16.77169
H	11.61756	0.66354	16.59637
H	15.4129	14.45295	17.12966
H	13.29023	1.11805	7.41017
H	17.5039	15.0907	7.04675
H	3.6878	15.28787	9.26886
H	0.63906	1.42919	8.36476
H	10.1932	14.63388	10.36162
H	9.37563	13.63904	9.14759

H	16.44191	13.82372	8.92477
H	15.20025	14.41207	7.80729
H	7.68696	14.95461	10.39512
H	5.3509	1.08197	10.04861
H	7.19472	14.63872	7.99099
H	3.42199	0.8594	8.51174
H	7.4735	14.08114	13.69088
H	7.18183	12.79041	12.52541
H	8.02038	0.98517	12.77565
H	7.5784	1.97258	14.17501
H	4.94629	1.869	14.96116
H	3.8555	0.94383	13.93188
H	14.73692	14.41412	4.94747
H	13.75596	13.45489	6.05126
H	14.86681	0.13396	0.87688
H	3.39084	14.06306	17.42124
H	13.02967	10.76097	3.40905
H	12.57993	11.21163	5.05373
H	11.36793	14.71587	8.127
H	7.60648	0.93506	8.65186
H	10.68493	0.34162	1.49114
H	13.02637	14.20803	1.14885
H	8.17752	0.63664	1.47812
H	8.97706	1.64761	0.26395
H	15.98901	7.55496	16.08616
H	15.72342	6.37504	17.40409
H	2.43713	7.0333	17.12158
H	3.63482	7.51953	2.52958
H	16.23713	6.24717	4.46309
H	2.82846	5.62721	5.18465
H	2.78096	7.26806	4.47151
H	2.48602	3.68822	15.41461
H	3.43031	4.66749	16.59794
H	1.8333	4.01842	17.05213
H	3.02616	4.01885	1.87744
H	2.66965	3.68502	3.60867
H	1.37484	4.26229	2.52567
H	8.67485	2.88192	11.10044
H	9.66926	2.87515	13.21836
H	10.01252	4.4839	12.55281
H	8.7723	4.2969	13.80503
H	3.17203	0.29446	4.42811
H	7.70335	14.63332	4.9895
H	6.24821	14.89447	5.99841
H	16.68888	13.69473	3.84405
H	17.63622	15.09511	3.32805
H	16.50203	14.30839	2.19536
H	9.57359	12.88479	13.2426
H	10.48953	11.51948	13.90263

H	9.15185	11.21255	12.78343
H	11.13792	0.60632	13.63309
H	12.64294	0.2586	14.54462
H	15.56169	14.86218	12.99187
H	8.96465	12.28122	4.64741
H	8.58714	10.69752	3.94091
H	9.89722	10.84394	5.12984
H	2.05564	1.05155	10.62604
H	1.9269	1.6025	12.3042
H	0.96263	0.21604	11.76201
H	8.10212	3.89287	5.24465
H	9.41011	4.17608	4.08945
H	8.97414	2.51304	4.55743

Table S5. Optimized geometry for (*SSSS*)-*PP* in the crystal state.

Cl	9.47138	4.34298	16.28535
Cl	7.39683	11.05829	10.51384
Cl	10.85966	4.17607	1.66296
Cl	6.58128	3.34835	16.52131
Cl	9.30199	11.03942	7.6838
Cl	4.4691	11.70336	9.82207
Cl	13.74179	3.44447	0.87502
Cl	12.20129	12.02046	7.72951
O	4.2302	3.86388	6.39729
O	14.12594	4.5296	10.6168
O	4.2734	10.72811	2.05683
O	9.39251	6.25807	5.36122
O	10.79551	8.94355	4.00526
O	3.99869	14.1178	5.16232
O	7.40455	3.20315	9.3237
O	9.16889	9.137	14.02305
O	8.22513	12.07418	17.45621
O	14.43733	11.39176	15.10258
O	14.74644	1.19798	13.73008
O	10.95231	12.0265	0.58991
O	7.94189	6.28321	12.70608
O	12.86577	14.68293	12.27885
O	5.85961	0.60445	3.57111
O	10.52105	3.28583	8.70874
O	3.78276	6.12315	1.02361
O	1.65244	4.86069	13.51794
N	13.68431	13.08795	13.74675
N	7.79399	4.72131	11.00654
N	14.46626	2.84329	12.12709
N	10.71762	10.49798	2.29306
N	8.66696	10.6452	15.70259
N	4.10518	12.45092	3.56068
N	5.04288	2.16837	5.07224

N	9.99901	4.73115	6.9915
N	1.78246	5.62638	15.69525
N	2.81639	5.71105	3.07632
C	4.97107	3.51759	5.46846
C	6.00808	9.21046	3.74776
C	12.02957	8.75049	11.65258
C	12.67403	6.77138	14.77001
C	7.36357	4.37298	9.71724
C	6.85554	5.44459	8.84729
C	12.33709	8.45059	12.99795
C	13.93102	4.08781	11.75377
C	5.97605	8.48815	6.09448
C	11.55843	8.44022	0.4995
C	6.42278	3.65485	0.65412
C	14.0396	2.96733	15.81283
C	10.72115	6.91699	8.67072
C	6.56657	5.21128	2.47489
C	6.1169	7.44878	7.05618
C	6.28349	6.83273	4.29301
C	13.18449	4.86556	12.77023
C	10.07477	7.16153	7.44553
C	13.88855	3.27939	14.47503
C	10.89166	5.58301	9.11699
C	12.4878	7.09133	13.40837
C	6.09368	4.20427	3.36763
C	6.12545	8.1854	4.7231
C	7.69492	6.0268	11.5279
C	6.51009	5.108	7.5611
C	12.39527	7.43195	17.11071
C	6.35699	7.80789	8.41428
C	6.54551	6.54863	2.93406
C	9.78372	6.03791	6.51047
C	6.52487	8.95288	2.42753
C	12.6081	9.48818	13.93236
C	6.1523	6.10147	6.63209
C	5.93531	2.88025	2.9034
C	12.44174	6.05353	17.5131
C	5.77523	4.5031	4.70997
C	11.03559	10.85508	0.97178
C	11.16572	7.99738	9.47899
C	12.541	9.15639	15.33885
C	6.75918	7.62084	2.02007
C	9.72211	8.46828	7.12768
C	12.58107	7.8029	15.74666
C	5.63263	1.78174	3.85581
C	10.88171	9.19336	2.80312
C	13.05827	13.49783	12.55917
C	4.57614	11.18453	3.16537
C	8.3013	10.91574	17.03741

C	8.85759	9.34393	15.19857
C	13.32291	4.52608	14.13092
C	14.39179	2.3413	13.4327
C	12.87931	10.77192	13.41873
C	6.06491	2.6292	1.54883
C	6.91732	10.01145	1.58758
C	11.99548	10.09222	11.20875
C	12.02094	11.67609	9.40534
C	6.29838	9.17924	8.83705
C	4.26311	12.95127	4.86447
C	11.74992	7.69155	10.74157
C	12.55188	6.07315	12.41933
C	11.18069	8.11626	1.81558
C	5.37304	10.40676	4.13769
C	6.0459	5.78517	5.22518
C	4.59508	12.26088	7.23674
C	5.69724	10.15109	7.90938
C	5.70626	9.8129	6.51373
C	14.44147	14.02806	14.63821
C	15.0634	15.20434	13.90647
C	13.64131	3.86175	16.82652
C	5.01589	11.3486	8.22668
C	13.71393	11.74142	14.1637
C	12.35176	15.19448	15.65405
C	5.27667	10.73186	5.50758
C	7.4369	5.98421	0.28067
C	11.4852	9.78715	0.06529
C	7.26661	7.10344	10.5851
C	4.72815	11.97731	5.88799
C	12.22761	10.14246	16.2921
C	11.60793	10.40599	9.86279
C	8.56771	11.84845	14.81912
C	9.48717	11.8498	13.60532
C	11.98176	6.35348	11.12702
C	7.05756	12.14229	14.57947
C	11.53633	3.2073	5.79691
C	8.0921	8.44031	17.41706
C	10.36299	11.66826	3.15476
C	9.40788	11.33995	4.29156
C	4.41022	12.44813	13.2816
C	8.68778	5.83684	16.64094
C	3.38516	13.20061	2.47582
C	17.23138	14.13605	2.99904
C	6.79782	6.78543	9.29696
C	8.97509	6.91256	15.78217
C	5.19535	0.91988	7.25235
C	6.94387	9.45657	10.06759
C	10.04197	3.52652	6.10524
C	9.08801	3.5448	4.92107

C	10.96469	9.35559	9.07024
C	4.34317	1.2097	5.99735
C	6.95584	15.36797	5.30642
C	11.38259	5.76508	1.24246
C	4.39768	13.84318	1.49147
C	11.04615	6.77705	2.16233
C	8.18715	3.53886	11.83656
C	9.21083	3.83036	12.92245
C	6.15058	10.93269	14.30423
C	10.0914	9.53296	7.96806
C	6.90432	2.79436	12.28621
C	8.64355	8.21264	16.14304
C	7.25663	7.33612	0.71719
C	10.44309	4.44767	8.2998
C	13.61813	14.36693	15.89723
C	12.66908	12.4117	11.62562
C	11.51457	5.30872	10.30954
C	7.46621	9.75692	0.35412
C	12.51886	11.08633	12.08936
C	2.5796	0.68149	0.06543
C	6.86235	4.91929	1.10258
C	14.03603	2.99685	4.2175
C	12.45309	12.68408	10.28697
C	13.1171	0.61792	10.70632
C	13.1054	1.79315	4.36507
C	7.38179	8.44152	10.94188
C	11.36376	13.63121	4.45464
C	6.48258	15.23948	1.15252
C	11.65047	12.45186	3.51948
C	5.47719	14.69059	2.16805
C	5.79857	3.65746	12.90682
C	11.65849	2.18527	4.6645
C	15.18208	2.14037	11.00789
C	1.35668	1.19138	11.46315
C	13.8909	3.973	5.38194
C	5.96058	0.74856	13.41414
C	4.52626	2.8189	13.06523
C	6.4682	0.10199	7.01387
C	12.43336	4.42301	5.51903
C	14.15323	1.5191	10.02847
C	4.68338	11.37747	14.33838
C	16.39665	5.73107	14.37927
C	5.38281	13.6259	13.38141
C	12.59564	14.53514	4.57948
C	12.08058	0.10124	9.70608
C	14.07512	12.51017	4.13541
C	5.15054	15.24127	16.91802
C	11.55982	15.35203	16.95707
C	14.49645	15.04627	16.96058

C	13.80039	0.253	7.86799
C	14.83583	0.77116	8.87201
C	9.61833	14.68192	9.42209
C	15.95309	14.74079	8.54313
C	5.1131	0.08447	9.64289
C	4.33079	0.25604	8.33876
C	6.84838	13.19832	13.49286
C	7.21466	1.60465	13.20027
C	4.76446	1.56771	13.91586
C	13.8514	13.75903	4.99557
C	3.68432	14.66684	0.40555
C	12.82498	11.62562	4.06033
C	10.46656	15.31922	8.31626
C	13.2578	15.20727	0.74161
C	8.74446	0.59991	0.53317
C	16.43397	6.70722	16.62655
C	3.44173	6.48895	2.15527
C	2.41196	6.23771	4.36788
C	2.42473	4.43007	16.21883
C	2.45088	4.34204	2.75376
C	12.93684	5.4373	15.1616
C	12.98202	5.07975	16.55116
H	14.52234	2.02756	16.08619
H	6.63072	4.0678	7.26721
H	9.69318	2.72496	6.7723
H	9.14988	8.66863	6.22163
H	5.85241	1.63292	1.16098
H	6.82869	11.04892	1.90335
H	4.11794	13.1935	7.54043
H	11.72344	14.72169	14.88288
H	9.42381	0.81307	15.25755
H	12.10409	11.18655	16.01345
H	6.6994	12.57746	15.5309
H	11.9339	2.73871	6.71556
H	3.37266	12.81482	13.35563
H	4.51151	11.97555	12.29156
H	9.46159	6.7285	14.8241
H	5.50658	1.90072	7.6564
H	15.66133	2.9748	10.47389
H	4.9101	13.00499	0.98319
H	10.6339	6.5154	3.14063
H	6.38922	10.4885	13.32178
H	6.3007	10.14168	15.05439
H	6.48247	2.37521	11.35655
H	13.29976	13.39963	16.32758
H	11.59648	4.26863	10.61696
H	2.12914	1.58577	0.51854
H	3.77278	1.04493	16.84419
H	15.27206	13.3968	14.9892

H	13.77551	3.54557	3.29778
H	15.07865	2.65494	4.10766
H	12.64929	13.68563	9.90389
H	12.60437	1.17144	11.50653
H	16.83005	15.13981	11.1905
H	9.81603	12.31936	2.45589
H	13.11524	1.20216	3.43906
H	13.48856	1.1356	5.16162
H	7.84894	8.7062	11.89409
H	10.50696	14.2197	4.09162
H	11.08983	13.24984	5.45324
H	8.9255	12.65659	15.4744
H	7.02429	14.39554	0.69062
H	4.03652	0.46711	1.67696
H	11.9915	12.88378	2.56183
H	1.79716	0.1525	2.71104
H	6.01084	14.09165	2.92096
H	6.12363	4.06345	13.88084
H	5.57327	4.53	12.27342
H	11.07413	1.28389	4.90457
H	11.21496	2.60881	3.75106
H	14.20797	3.48998	6.32439
H	14.54725	4.84679	5.23955
H	9.38914	15.30551	14.11881
H	5.69679	0.27238	12.45442
H	4.19233	2.51241	12.05762
H	3.7094	3.42974	13.47736
H	9.40687	14.48155	6.6157
H	7.09298	0.58324	6.2437
H	12.10993	4.93592	4.59514
H	12.36146	5.16091	6.33257
H	13.60406	2.36671	9.58033
H	4.01608	10.51306	14.19133
H	4.46148	11.77898	15.34446
H	3.49578	1.81418	6.35543
H	15.93507	6.71662	14.13643
H	2.88744	12.39191	1.91867
H	5.27345	14.27183	12.50127
H	5.11425	14.25077	14.24749
H	12.39288	15.33962	5.30703
H	12.77077	15.02804	3.60783
H	11.4978	0.95591	9.31971
H	14.56549	14.82429	10.2266
H	14.93234	11.93269	4.51996
H	14.34098	12.81971	3.10821
H	5.62418	14.40129	16.38148
H	1.42121	0.46222	16.1541
H	11.2166	14.35937	17.29065
H	7.45498	0.58139	16.77169

H	11.61756	0.66354	16.59637
H	15.4129	14.45295	17.12966
H	13.29023	1.11805	7.41017
H	17.5039	15.0907	7.04675
H	3.6878	15.28787	9.26886
H	0.63906	1.42919	8.36476
H	10.1932	14.63388	10.36162
H	9.37563	13.63904	9.14759
H	16.44191	13.82372	8.92477
H	15.20025	14.41207	7.80729
H	7.68696	14.95461	10.39512
H	5.3509	1.08197	10.04861
H	7.19472	14.63872	7.99099
H	3.42199	0.8594	8.51174
H	7.4735	14.08114	13.69088
H	7.18183	12.79041	12.52541
H	8.02038	0.98517	12.77565
H	7.5784	1.97258	14.17501
H	4.94629	1.869	14.96116
H	3.8555	0.94383	13.93188
H	14.73692	14.41412	4.94747
H	13.75596	13.45489	6.05126
H	14.86681	0.13396	0.87688
H	3.39084	14.06306	17.42124
H	13.02967	10.76097	3.40905
H	12.57993	11.21163	5.05373
H	11.36793	14.71587	8.127
H	7.60648	0.93506	8.65186
H	10.68493	0.34162	1.49114
H	13.02637	14.20803	1.14885
H	8.17752	0.63664	1.47812
H	8.97706	1.64761	0.26395
H	15.98901	7.55496	16.08616
H	15.72342	6.37504	17.40409
H	2.43713	7.0333	17.12158
H	3.63482	7.51953	2.52958
H	16.23713	6.24717	4.46309
H	2.82846	5.62721	5.18465
H	2.78096	7.26806	4.47151
H	2.48602	3.68822	15.41461
H	3.43031	4.66749	16.59794
H	1.8333	4.01842	17.05213
H	3.02616	4.01885	1.87744
H	2.66965	3.68502	3.60867
H	1.37484	4.26229	2.52567
H	8.67485	2.88192	11.10044
H	9.66926	2.87515	13.21836
H	10.01252	4.4839	12.55281
H	8.7723	4.2969	13.80503

H	3.17203	0.29446	4.42811
H	7.70335	14.63332	4.9895
H	6.24821	14.89447	5.99841
H	16.68888	13.69473	3.84405
H	17.63622	15.09511	3.32805
H	16.50203	14.30839	2.19536
H	9.57359	12.88479	13.2426
H	10.48953	11.51948	13.90263
H	9.15185	11.21255	12.78343
H	11.13792	0.60632	13.63309
H	12.64294	0.2586	14.54462
H	15.56169	14.86218	12.99187
H	8.96465	12.28122	4.64741
H	8.58714	10.69752	3.94091
H	9.89722	10.84394	5.12984
H	2.05564	1.05155	10.62604
H	1.9269	1.6025	12.3042
H	0.96263	0.21604	11.76201
H	8.10212	3.89287	5.24465
H	9.41011	4.17608	4.08945
H	8.97414	2.51304	4.55743

Table S6. TDDFT calculations on $\boldsymbol{\mu}$, $\boldsymbol{m}$, and the angel of the two vectors (θ) of *SSSS-PP* in monomers.

Excited States	oscillator strength	$\lvert R_{vel}\rvert$	$\lvert\boldsymbol{\mu}_e\rvert$ (10^{-20} esu·cm)	$\lvert\boldsymbol{\mu}_m\rvert$ (10^{-20} erg·G^{-1})	θ (°)	$\lvert g_{abs}\rvert$
1	0.4401	442.22	811.20	0.53	2.76	0.0026
2	0.0208	169.07	160.77	1.04	180.00	0.0257
3	0.1090	611.81	351.17	1.70	179.74	0.0194
4	0.4622	97.13	722.99	0.18	141.08	0.0008
5	0.0192	136.25	138.55	0.99	0.01	0.0286
6	0.6347	471.80	765.91	0.81	40.61	0.0032
7	0.0038	15.45	58.86	0.29	26.62	0.0179
8	0.0021	7.96	43.60	0.17	0.13	0.0158
9	0.0174	41.24	124.18	0.40	149.05	0.0111
10	0.0000	0.23	1.32	0.05	179.00	0.1555
11	0.0027	58.45	48.24	1.24	0.11	0.1025
12	0.2593	2.25	471.16	0.39	91.49	0.0001
13	0.0051	33.74	65.55	0.49	0.11	0.0300
14	0.0004	2.34	18.89	0.21	4.18	0.0442
15	0.0000	0.47	2.96	0.20	4.16	0.2675
16	0.0014	34.23	34.80	0.96	0.33	0.1101
17	0.0032	10.82	51.39	0.35	178.76	0.0269
18	0.0702	34.30	241.21	0.23	49.08	0.0025
19	0.0032	32.19	51.47	0.63	0.06	0.0487
20	0.0389	3.18	176.84	0.08	78.39	0.0004
21	0.0458	6.22	191.65	0.30	98.47	0.0009
22	0.0035	6.46	52.61	0.14	179.97	0.0104

23	0.0004	9.71	18.61	0.49	0.56	0.1052
24	0.0065	3.23	71.20	0.21	79.22	0.0022
25	0.0350	2.30	165.03	0.10	99.05	0.0004
26	0.0030	2.09	47.84	0.05	179.95	0.0039
27	0.1078	104.20	286.56	0.61	130.91	0.0056
28	0.0002	20.84	12.3	1.49	179.84	0.4768
29	0.3653	182.30	522.72	0.39	154.22	0.0027
30	0.0080	28.01	76.86	0.38	0.06	0.0195
31	0.0738	2.29	232.67	0.21	90.51	0.0000
32	0.0473	48.11	185.07	0.31	151.72	0.0059
33	0.0007	24.22	22.42	1.01	0.48	0.1793
34	0.0080	44.80	75.67	0.63	0.14	0.0333
35	0.0273	5.38	140.04	0.13	107.45	0.0011
36	0.0042	70.69	54.52	1.28	179.92	0.0940
37	0.0001	4.65	9.05	0.44	179.65	0.1919
38	0.0180	7.33	113.00	0.30	80.64	0.0017
39	0.0001	4.51	7.91	0.70	0.53	0.3500
40	0.0096	12.56	82.26	0.19	31.89	0.0078
41	0.0000	0.27	0.45	0.11	116.23	0.3948
42	0.0244	49.66	130.72	0.41	3.21	0.0125
43	0.0189	34.65	114.68	0.29	179.99	0.0102
44	0.0136	33.67	97.35	0.47	143.58	0.0155
45	0.0363	35.74	158.32	0.26	171.01	0.0065
46	0.0037	19.30	50.04	50.05	0.15	0.0312
47	0.0310	10.63	145.15	0.16	118.71	0.0021
48	0.0023	0.02	39.68	0.00	8.13	0.0001
49	0.0076	10.12	71.34	0.20	148.29	0.0093
50	0.0013	28.86	29.64	0.95	179.95	0.1286
51	0.0000	1.55	2.77	0.55	1.64	0.7692
52	0.0156	8.925	101.61	0.22	117.11	0.0039
53	0.0020	0.75	36.71	0.02	3.57	0.0024
54	0.0017	3.71	33.64	0.31	75.89	0.0089
55	0.0612	53.69	53.69	0.34	143.79	0.0055
56	0.0021	31.38	31.38	0.91	179.93	0.0972
57	0.0039	0.79	50.45	0.02	179.40	0.0014
58	0.0142	21.24	96.11	0.29	138.61	0.0091
59	0.0002	0.38	11.97	0.04	179.26	0.0128
60	0.0012	0.53	27.69	0.03	125.91	0.0023

.

Table S7. TDDFT calculations on $\boldsymbol{\mu}$, $\boldsymbol{m}$, and the angel of the two vectors (θ) of *SSSS-MM* in crystals.

Excited States	oscillator strength	$\lvert R_{vel}\rvert$	$\lvert\boldsymbol{\mu_e}\rvert$ (10^{-20} esu·cm)	$\lvert\boldsymbol{\mu_m}\rvert$ (10^{-20} erg·G^{-1})	θ (°)	$\lvert g_{abs}\rvert$
1	0.3258	272.41	687.52	1.50	105.4658	0.0023
2	0.0001	1.08	10.00	0.12	27.91	0.0419
3	0.0013	1.24	41.31	0.30	93.19	0.0016
4	0.0013	10.32	41.16	0.37	48.09	0.0241
5	0.0151	128.16	136.21	1.15	38.59	0.0265
6	0.0045	6.18	72.94	0.18	119.33	0.0048
7	0.0108	7.28	110.60	0.16	115.12	0.0025

8	0.0342	35.73	194.29	0.85	80.08	0.0030
9	0.0550	43.97	245.89	0.61	73.30	0.0029
10	0.0289	117.56	177.62	1.13	55.41	0.0144
11	0.0724	213.59	279.96	1.27	54.58	0.0105
12	0.0575	57.05	249.50	0.87	75.43	0.0035
13	0.0004	1.31	19.65	0.22	99.59	0.0075
14	0.0235	38.70	155.09	0.68	112.37	0.0066
15	0.0015	0.57	38.74	0.14	94.15	0.0011
16	0.0013	3.28	35.47	0.11	159.55	0.0121
17	0.0043	30.87	64.52	0.48	162.56	0.0283
18	0.0047	8.76	67.10	0.17	142.03	0.0082
19	0.0015	3.73	28.23	0.41	100.36	0.0078
20	0.0023	3.71	46.22	0.19	114.27	0.0068
21	0.0017	10.10	39.39	0.50	121.82	0.0265
22	0.0067	23.39	78.26	0.46	126.79	0.0141
23	0.0124	10.76	106.60	0.25	112.96	0.0037
24	0.0176	24.34	126.04	0.40	114.54	0.0053
25	0.0038	7.07	58.52	0.64	98.53	0.0065
26	0.2459	173.37	467.83	1.17	108.90	0.0032
27	0.0076	11.713	82.00	0.56	104.07	0.0067
28	0.0251	21.69	148.88	0.52	104.24	0.0034
29	0.0518	21.12	212.99	0.95	97.08	0.0022
30	0.1190	58.00	322.34	1.10	98.09	0.0019
31	0.0065	89.38	74.71	1.26	152.03	0.0595
32	0.0117	10.22	100.20	0.52	97.75	0.0028
33	0.0029	6.00	49.82	0.14	136.85	0.0081
34	0.0064	13.74	73.33	0.54	108.17	0.0093
35	0.0062	9.76	72.23	0.33	113.46	0.0073
36	0.0002	0.09	13.44	0.10	80.86	0.0046
37	0.0027	6.21	47.66	0.30	117.68	0.0117
38	0.0065	7.73	73.67	0.41	102.47	0.0048
39	0.0058	8.85	69.12	0.19	48.54	0.0071
40	0.2254	94.11	430.23	1.40	97.77	0.0018
41	0.0104	35.06	92.14	0.64	130.04	0.0180
42	0.0090	1.32	86.17	0.46	86.52	0.0013
43	0.0157	14.82	112.33	0.55	105.89	0.0054
44	0.0128	22.58	101.35	0.44	59.02	0.0090
45	0.0178	27.80	117.29	0.81	71.65	0.0088
46	0.0043	7.32	57.65	0.18	135.14	0.0089
47	0.0007	1.74	23.73	23.73	63.59	0.0093
48	0.0034	3.69	51.31	0.30	70.24	0.0079
49	0.0273	15.11	144.26	0.42	74.03	0.0032
50	0.0455	7.40	186.06	0.71	93.07	0.0008
51	0.0067	9.65	71.40	0.33	112.54	0.0071
52	0.0160	15.77	109.86	0.38	64.25	0.0060
53	0.0590	0.53	210.53	1.17	87.89	0.0008
54	0.0004	5.27	16.55	0.60	59.65	0.0729
55	0.0019	12.67	37.45	0.85	67.78	0.0342
56	0.0509	9.56	194.75	0.50	83.71	0.0011
57	0.0109	1.56	89.77	0.58	90.85	0.0004
58	0.0030	1.35	47.36	0.38	95.11	0.0029
59	0.0264	22.50	139.58	0.75	76.04	0.0052
60	0.0266	11.81	139.94	0.33	74.39	0.0025

6. Estimation of Chiro-optical and Electrical Properties

The field−effect mobility (μ) and the threshold voltage (V_T) were estimated in the saturation regime (V_{DS} = −100 V) with the following equation:

$$I_D = \frac{W}{2L}\mu C_i (V_G - V_T)^2 \quad \text{(S1)}$$

where I_D is the drain current, W and L are the semiconductor channel width and length, respectively. μ is the mobility and C_i is the capacitance per unit area of the gate dielectric. V_G and V_T are the gate voltage and threshold voltage, respectively.

In order to investigate photosensitivity for OPTs, photoresponsivity (R) and the ratio of photocurrent to dark current (P) were calculated from transfer characteristics coupled with light irradiation. The R and P values are typically defined by the following equations:

$$R = \frac{I_{ph}}{P_{inc}} = \frac{I_{light} - I_{dark}}{P_{inc}} \quad \text{(S2)}$$

$$P = \frac{(I_{light} - I_{dark})}{I_{dark}} \quad \text{(S3)}$$

where I_{ph} is the photocurrent, P_{inc} the incident illumination power on the channel of the device, I_{light} the drain current under illumination, and I_{dark} the drain current in the dark, respectively.

In addition, the external quantum efficiency (EQE) (η) of OPTs was calculated which can be defined as the ratio of number of photogenerated carriers that practically enhances the drain current to the number of photons incident onto the OPT channel area, using the following equation:

$$\eta = \frac{(I_{light} - I_{dark})hc}{eP_{inc}A\lambda_{peak}} \quad \text{(S4)}$$

where h is the plank constant, c the speed of light, e the fundamental unit of charge, A the area of the transistor channel, and λ_{peak} the peak wavelength of the incident light, respectively.

Table S8. Charge transport performances of thin-film and single crystal based transistors.

	μ_{avg} (cm^2 V^{-1} s^{-1})	V_{th} (V)	I_{on}/I_{off}
Single crystals	6.07×10^{-2}	−6.7	1.1×10^3
Thin films	4.78×10^{-4}	−9.3	2.1×10^3

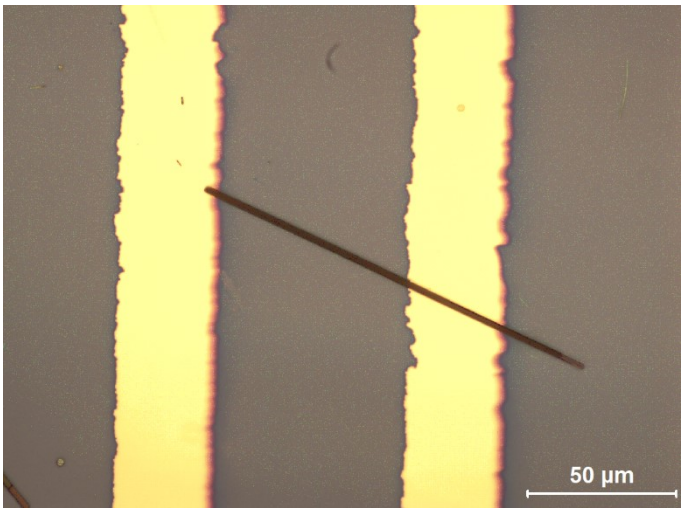


Figure S13. Optical microscope image of NWs-based OPTs.

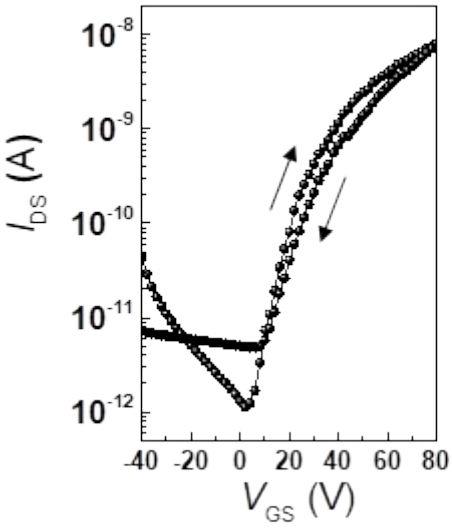


Figure S14. I_{DS}-V_{GS} hysteresis characteristics of (*SSSS*)-4CldiPDI NWs. The sweep directions are indicated by the arrows.

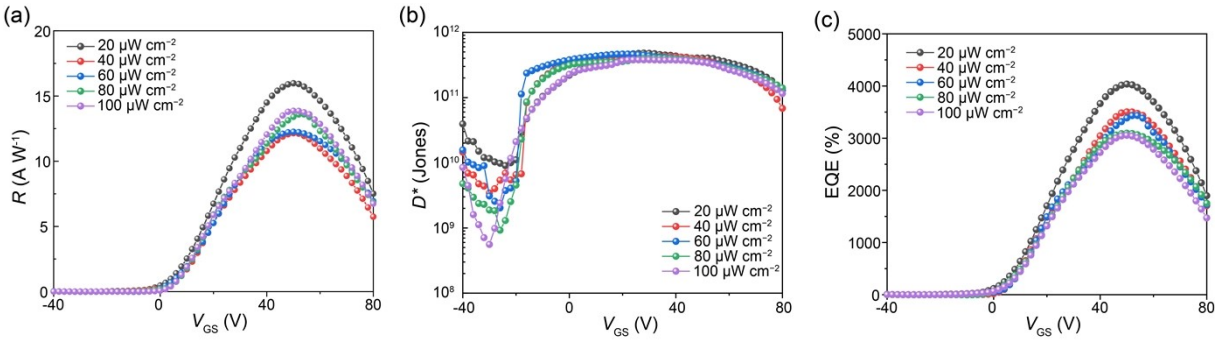


Figure S15. (a-c) Optoelectronic performances of (*SSSS*)-4CldiPDI NWs under various light intensities. *R*, *D**, EQE values were plotted as a function of V_{GS} under monxqochromatic light (λ = 488 nm) irradiation at V_D = 80 V, with intensities ranging from 20 to 100 μW cm^{-2}.

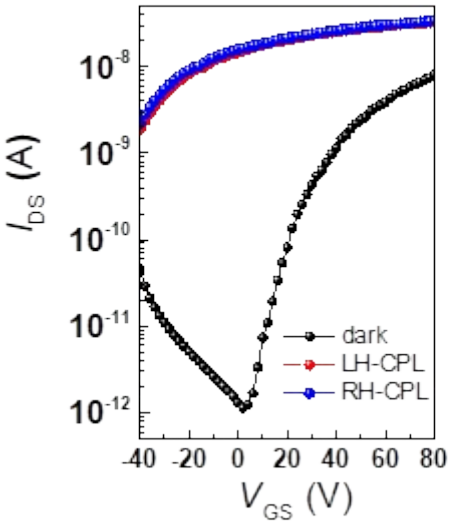


Figure S16. I_{DS}-V_{GS} characteristics of (*SSSS*)-4CldiPDI NWs under dark and CPL illumination (λ = 488 nm).

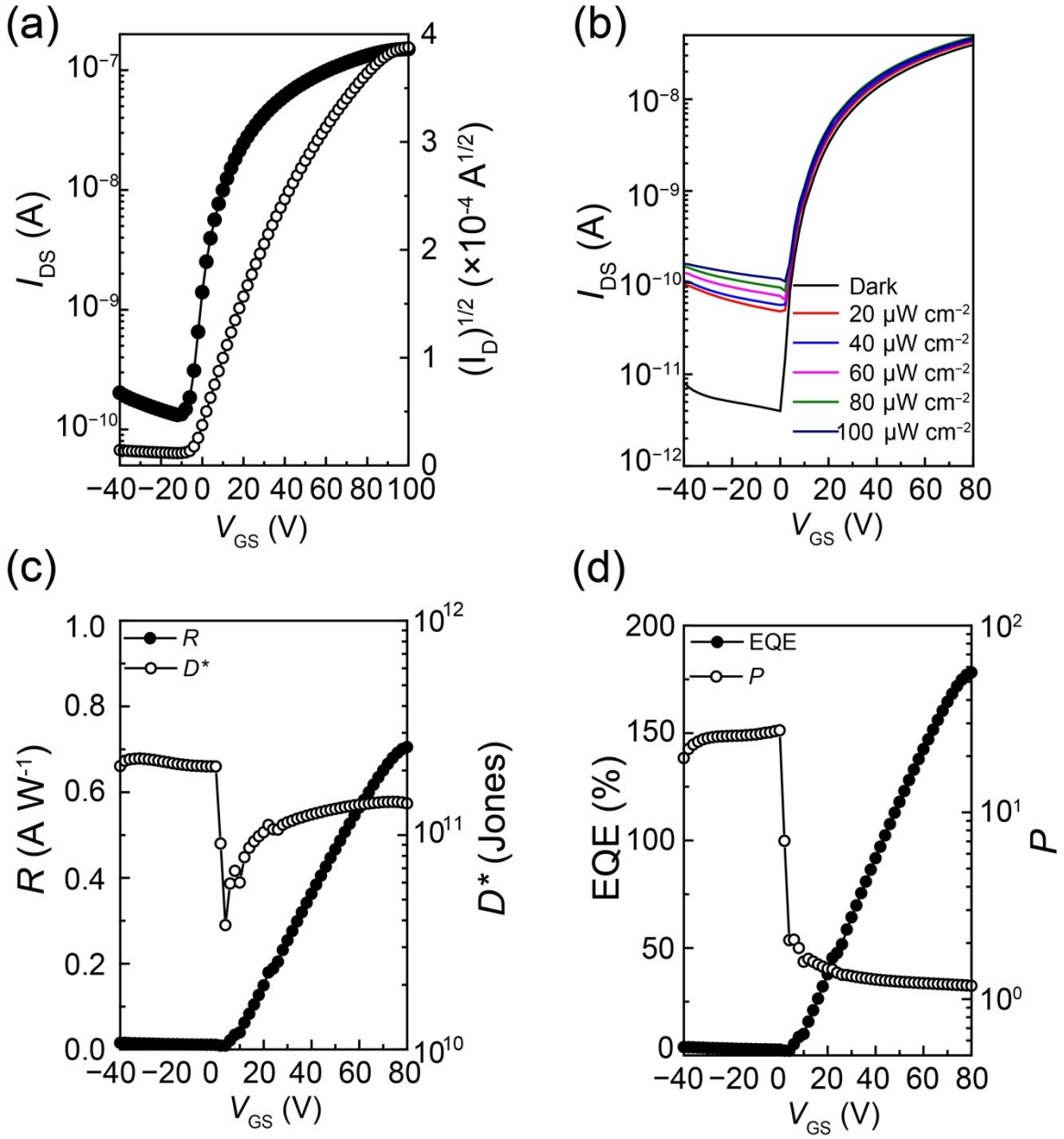


Figure S17. (a) I_{DS}-V_{GS} characteristics and in the dark of (*SSSS*)-4CldiPDI thin films. (b) I_{DS}–V_{GS} characteristics of (*SSSS*)-4CldiPDI thin films under dark and monochromatic light illumination (λ = 488 nm) of various intensities and under vacuum. (c-d) Optoelectronic performances for the (*SSSS*)-4CldiPDI thin films. Photoresponsivity (*R*), specific detectivity (D^*), external quantum efficiency (EQE), and photo to dark current ratio (*P*) values were plotted as a function of V_{GS} under monochromatic light (λ = 488 nm) irradiation at V_D = 100 V, with an intensity of 20 μW cm^{-2}.

7. References:

[S1] Queste, M.; Cadiou, C.; Pagoaga, B.; Giraudetc, L.; Hoffmann, N. *New J. Chem.* **2010**, *34*, 2537−2545.

[S2] Frisch, G.; Robb, J.; Nakatsuji, MC.; Sonnenberg, M.; Farkas, JBF. Gaussian, Inc., Wallingford CT, **2016**.

[S3] AD, Becke. *J. Chem. Phys.* **1993**, *98*, 5648−5652.

[S4] PC, Hariharan.; JA, Pople.; *Mol. Phys.* **1974**, *27*, 209−214.

[S5] O'Boyle, N.M.; Vandermeersch, T.; Flynn, C.J.; Maguire, A. R.; Hutchison, G. R. *J Cheminform*, **2011**, *3*, 8.

[S6] Bannwarth, C.; Caldeweyher, E.; Ehlert, S.; Hansen, A.; Pracht, P.; Seibert, J.; Spicher, S.; Grimme, S. *WIREs Comput Mol Sci*. **2021**, 11, e1493.

[S7] Kresse, G.; Furthmüller, J.; *Comput. Mater. Sci.* **1996**, *6*, 15−50.

[S8] Kresse, G.; Furthmüller, J. *Phys. Rev. B* **1996**, *54*, 11169−11186.

[S9] Blochl, P. E. *Phys. Rev. B* **1994**, *50*, 17953−17979.

[S10] Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, *77*, 3865−3868.

[S11] Bruker, *SAINT*, *V8.40B*, Bruker AXS Inc., Madison, Wisconsin, USA.

[S12] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.* **2015**, *48*, 3–10.

[S13] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3–8.

[S14] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3–8.

[S15] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339–341.